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(54) **CRYSTALS OF GLUCOKINASE AND METHODS OF GROWING THEM**

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(52) **U.S. Cl.** **546/270.7**
(58) **Field of Search** 546/270.7

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(57) **ABSTRACT**

Crystalline forms of mammalian Gluckokinase of sufficient size and quality to obtain structural data by X-ray crystallography are presented. Methods of growing such crystals are also disclosed.

1 Claim, 65 Drawing Sheets

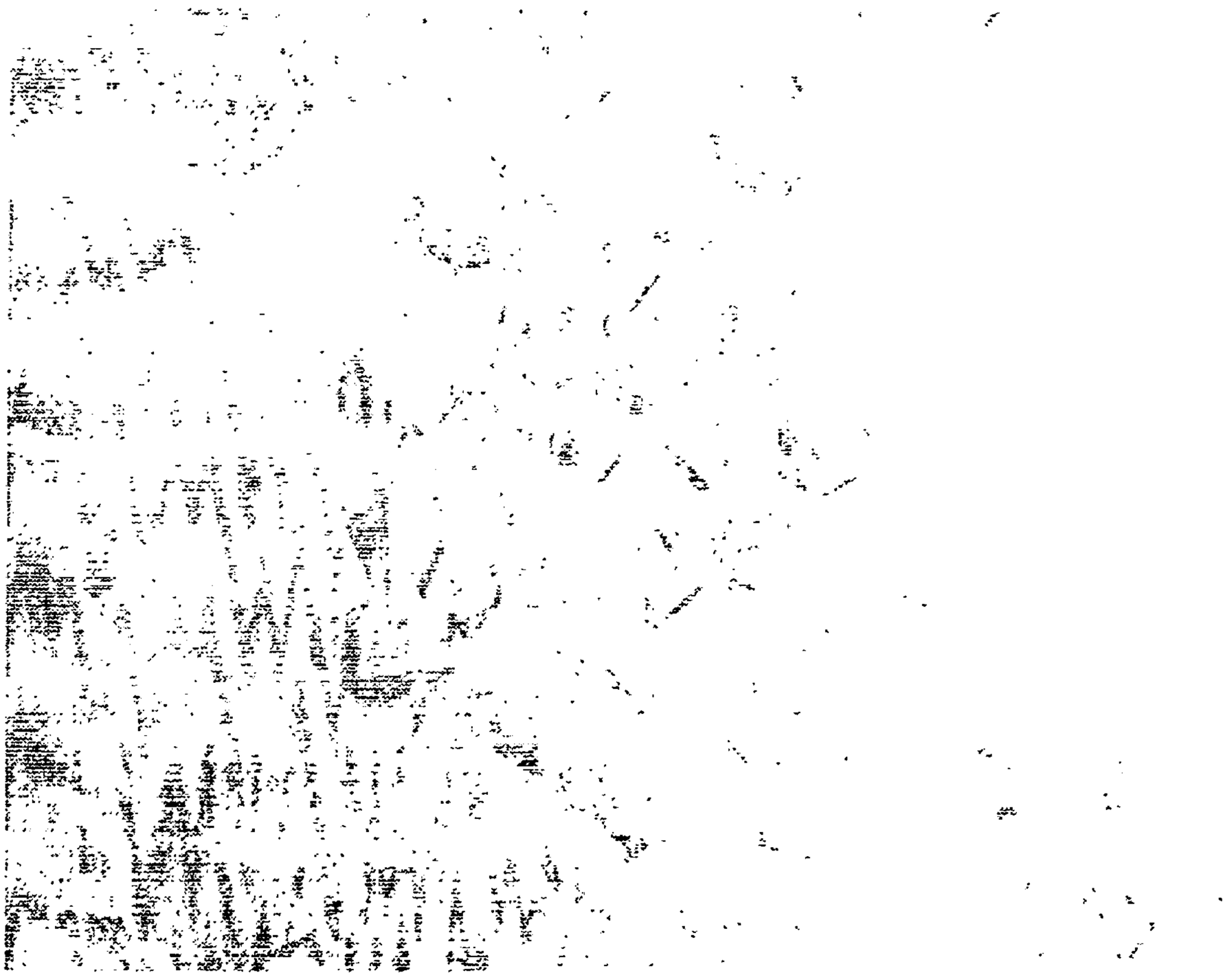

Figure 1

Figure 2. The amino-acid sequence of the GST-GK fusion protein. The GST sequence was taken from GenBank entry U13852. Residue 229 of the fusion protein is the first residue of GK.

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  1 MSPILGYWKI KGLVQPTRLL LEYLEEKYEE HLYERDEGDK WRNKKFELGL EFPNLPYYID
 61 GDVKLTQSMA IIRYIADKHN MLGGCPKERA EISMLEGAVL DIRYGVSRIA YSKDFETLKV
121 DFLSKLPEML KMFEDRLCHK TYLNGDHVTH PDFMLYDALD VVLYMDPMCL DAFPKLVCFK
181 KRIEAIPQID KYLKSSKYIA WPLQGWQATF GGGDHPPKSD LIEGRGIHMP RPRSQLPQPN
241 SQVEQILAEF QLQEEDLKKV MRRMQKEMDR GLRLETHEEA SVKMLPTYVR STPEGSEVGD
301 FLSLDLGGTN FRVMLVKVGE GEEGQWSVKT KHQMYSIPED AMTGTAEMLF DYISECISDF
361 LDKHQMKHKK LPLGFTFSFP VRHEDIDKGI LLNWTKGFKA SGAEGNNVVG LLRDAIKRRG
421 DFEMDVVAMV NDTVATMISC YYEDHQCEVG MIVGTGCNAC YMEEMQNVEL VEGDEGRMCV
481 NTEWGAFGDS GELDEFLLEY DRLVDESSAN PGQQLYEKLI GGKYMGELVR LVLLRLVDEN
541 LLFHGEASEQ LRTRGAFETR FVSQVESDTG DRKQIYNILS TLGLRPSTTD CDIVRRACES
601 VSTRAAHMCS AGLAGVINRM RESRSEDVMR ITVGVDGSVY KLHPSFKERF HASVRRLTPS
661 CEITFIESEE GSGRGAALVS AVACKKACML GQ
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Figure 3

Atom	No.	Atom Type	A.A. Type	A.A.#	X	Y	Z	OCC	B
ATOM	1	CB	SER	8	-0.421	63.744	24.899	1.00	50.68
ATOM	2	OG	SER	8	-0.752	63.605	23.524	1.00	50.85
ATOM	3	C	SER	8	1.865	64.216	24.094	1.00	50.72
ATOM	4	O	SER	8	2.308	63.644	23.102	1.00	51.79
ATOM	5	N	SER	8	1.473	63.793	26.507	1.00	50.36
ATOM	6	CA	SER	8	1.057	63.446	25.120	1.00	50.55
ATOM	7	N	GLN	9	2.041	65.515	24.314	1.00	49.84
ATOM	8	CA	GLN	9	2.831	66.312	23.385	1.00	48.95
ATOM	9	CB	GLN	9	2.983	67.745	23.895	1.00	49.08
ATOM	10	CG	GLN	9	3.676	68.686	22.925	1.00	50.25
ATOM	11	CD	GLN	9	3.206	70.127	23.085	1.00	51.06
ATOM	12	OE1	GLN	9	2.037	70.433	22.846	1.00	51.38
ATOM	13	NE2	GLN	9	4.112	71.017	23.499	1.00	51.44
ATOM	14	C	GLN	9	4.190	65.633	23.294	1.00	48.56
ATOM	15	O	GLN	9	4.884	65.741	22.285	1.00	48.75
ATOM	16	N	VAL	10	4.560	64.926	24.361	1.00	47.77
ATOM	17	CA	VAL	10	5.823	64.198	24.392	1.00	46.87
ATOM	18	CB	VAL	10	6.293	63.902	25.842	1.00	46.39
ATOM	19	CG1	VAL	10	7.303	62.782	25.841	1.00	46.41
ATOM	20	CG2	VAL	10	6.952	65.135	26.436	1.00	46.79
ATOM	21	C	VAL	10	5.616	62.885	23.653	1.00	46.17
ATOM	22	O	VAL	10	6.521	62.384	22.991	1.00	46.18
ATOM	23	N	GLU	11	4.423	62.317	23.768	1.00	45.28
ATOM	24	CA	GLU	11	4.159	61.071	23.069	1.00	45.19
ATOM	25	CB	GLU	11	2.905	60.393	23.616	1.00	45.21
ATOM	26	CG	GLU	11	3.105	59.709	24.967	1.00	46.05
ATOM	27	CD	GLU	11	4.224	58.664	24.957	1.00	46.30
ATOM	28	OE1	GLU	11	4.350	57.918	23.948	1.00	46.28
ATOM	29	OE2	GLU	11	4.963	58.583	25.972	1.00	45.66
ATOM	30	C	GLU	11	4.002	61.345	21.580	1.00	44.48
ATOM	31	O	GLU	11	4.068	60.430	20.755	1.00	44.48
ATOM	32	N	GLN	12	3.807	62.614	21.239	1.00	43.86
ATOM	33	CA	GLN	12	3.646	62.996	19.845	1.00	42.86
ATOM	34	CB	GLN	12	2.972	64.368	19.715	1.00	44.49
ATOM	35	CG	GLN	12	2.833	64.840	18.259	1.00	46.49
ATOM	36	CD	GLN	12	1.986	66.099	18.113	1.00	47.74
ATOM	37	OE1	GLN	12	2.055	66.799	17.088	1.00	48.30
ATOM	38	NE2	GLN	12	1.174	66.388	19.131	1.00	47.51
ATOM	39	C	GLN	12	5.014	63.023	19.192	1.00	41.14
ATOM	40	O	GLN	12	5.139	62.739	18.002	1.00	41.76
ATOM	41	N	ILE	13	6.038	63.360	19.971	1.00	38.51
ATOM	42	CA	ILE	13	7.398	63.388	19.450	1.00	36.48
ATOM	43	CB	ILE	13	8.274	64.351	20.261	1.00	35.85
ATOM	44	CG2	ILE	13	9.731	64.228	19.827	1.00	35.71
ATOM	45	CG1	ILE	13	7.740	65.777	20.079	1.00	35.77
ATOM	46	CD1	ILE	13	8.584	66.867	20.710	1.00	35.91
ATOM	47	C	ILE	13	8.018	61.981	19.452	1.00	36.01
ATOM	48	O	ILE	13	8.572	61.528	18.442	1.00	35.99
ATOM	49	N	LEU	14	7.903	61.288	20.580	1.00	34.88
ATOM	50	CA	LEU	14	8.430	59.934	20.711	1.00	33.91
ATOM	51	CB	LEU	14	8.230	59.432	22.141	1.00	33.29
ATOM	52	CG	LEU	14	8.853	60.321	23.215	1.00	33.43
ATOM	53	CD1	LEU	14	8.510	59.781	24.594	1.00	33.04

FIG. 4A

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ATOM     54  CD2 LEU   14      10.354  60.398  23.001  1.00 33.04
ATOM     55  C   LEU   14       7.766  58.957  19.730  1.00 33.55
ATOM     56  O   LEU   14       8.208  57.812  19.578  1.00 33.21
ATOM     57  N   ALA   15       6.710  59.403  19.065  1.00 32.69
ATOM     58  CA  ALA   15       6.021  58.551  18.104  1.00 32.59
ATOM     59  CB  ALA   15       4.628  59.104  17.821  1.00 31.95
ATOM     60  C   ALA   15       6.838  58.449  16.808  1.00 32.79
ATOM     61  O   ALA   15       6.664  57.519  16.018  1.00 33.05
ATOM     62  N   GLU   16       7.746  59.395  16.599  1.00 32.33
ATOM     63  CA  GLU   16       8.575  59.369  15.403  1.00 32.74
ATOM     64  CB  GLU   16       9.566  60.531  15.401  1.00 34.23
ATOM     65  CG  GLU   16       8.950  61.910  15.298  1.00 38.39
ATOM     66  CD  GLU   16      10.017  62.998  15.162  1.00 41.11
ATOM     67  OE1 GLU   16      10.445  63.269  14.012  1.00 40.68
ATOM     68  OE2 GLU   16      10.438  63.562  16.212  1.00 42.77
ATOM     69  C   GLU   16       9.369  58.073  15.279  1.00 31.93
ATOM     70  O   GLU   16       9.570  57.568  14.179  1.00 33.41
ATOM     71  N   PHE   17       9.841  57.539  16.401  1.00 30.37
ATOM     72  CA  PHE   17      10.640  56.321  16.369  1.00 27.71
ATOM     73  CB  PHE   17      11.346  56.129  17.711  1.00 26.32
ATOM     74  CG  PHE   17      12.309  57.230  18.045  1.00 24.22
ATOM     75  CD1 PHE   17      11.846  58.500  18.389  1.00 23.88
ATOM     76  CD2 PHE   17      13.680  57.010  17.981  1.00 22.24
ATOM     77  CE1 PHE   17      12.741  59.531  18.660  1.00 22.63
ATOM     78  CE2 PHE   17      14.574  58.027  18.250  1.00 21.23
ATOM     79  CZ  PHE   17      14.105  59.291  18.589  1.00 22.01
ATOM     80  C   PHE   17       9.836  55.077  16.012  1.00 27.77
ATOM     81  O   PHE   17      10.400  54.004  15.802  1.00 27.38
ATOM     82  N   GLN   18       8.517  55.213  15.957  1.00 28.12
ATOM     83  CA  GLN   18       7.684  54.080  15.593  1.00 29.17
ATOM     84  CB  GLN   18       6.216  54.484  15.599  1.00 30.98
ATOM     85  CG  GLN   18       5.446  54.017  16.806  1.00 32.94
ATOM     86  CD  GLN   18       4.152  54.785  16.974  1.00 34.65
ATOM     87  OE1 GLN   18       3.389  54.976  16.014  1.00 37.17
ATOM     88  NE2 GLN   18       3.892  55.228  18.190  1.00 33.67
ATOM     89  C   GLN   18       8.068  53.602  14.193  1.00 28.97
ATOM     90  O   GLN   18       8.471  54.399  13.346  1.00 28.83
ATOM     91  N   LEU   19       7.931  52.298  13.971  1.00 29.02
ATOM     92  CA  LEU   19       8.235  51.659  12.704  1.00 29.94
ATOM     93  CB  LEU   19       9.641  51.069  12.749  1.00 29.78
ATOM     94  CG  LEU   19      10.782  51.813  12.037  1.00 30.77
ATOM     95  CD1 LEU   19      10.886  53.251  12.477  1.00 30.67
ATOM     96  CD2 LEU   19      12.083  51.087  12.339  1.00 32.05
ATOM     97  C   LEU   19       7.199  50.549  12.511  1.00 31.41
ATOM     98  O   LEU   19       7.288  49.484  13.137  1.00 31.35
ATOM     99  N   GLN   20       6.205  50.801  11.663  1.00 32.64
ATOM    100  CA  GLN   20       5.153  49.817  11.422  1.00 34.95
ATOM    101  CB  GLN   20       4.024  50.413  10.570  1.00 35.78
ATOM    102  CG  GLN   20       3.301  51.622  11.175  1.00 37.65
ATOM    103  CD  GLN   20       3.048  51.486  12.669  1.00 39.03
ATOM    104  OE1 GLN   20       2.603  50.441  13.152  1.00 40.92
ATOM    105  NE2 GLN   20       3.324  52.552  13.410  1.00 40.04
ATOM    106  C   GLN   20       5.692  48.568  10.730  1.00 35.83
ATOM    107  O   GLN   20       6.827  48.547  10.247  1.00 36.56
ATOM    108  N   GLU   21       4.864  47.531  10.681  1.00 36.52
ATOM    109  CA  GLU   21       5.240  46.279  10.062  1.00 37.80
ATOM    110  CB  GLU   21       4.024  45.357   9.998  1.00 39.22
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FIG. 4B

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ATOM    111  CG  GLU    21       4.298  43.898   9.625  1.00 42.88
ATOM    112  CD  GLU    21       4.568  43.009  10.844  1.00 44.63
ATOM    113  OE1 GLU    21       4.540  41.758  10.699  1.00 45.40
ATOM    114  OE2 GLU    21       4.810  43.564  11.943  1.00 45.89
ATOM    115  C   GLU    21       5.770  46.549   8.654  1.00 38.20
ATOM    116  O   GLU    21       6.892  46.183   8.324  1.00 38.71
ATOM    117  N   GLU    22       4.972  47.208   7.826  1.00 38.54
ATOM    118  CA  GLU    22       5.386  47.478   6.457  1.00 39.08
ATOM    119  CB  GLU    22       4.308  48.267   5.703  1.00 40.61
ATOM    120  CG  GLU    22       3.123  47.406   5.313  1.00 43.51
ATOM    121  CD  GLU    22       3.556  46.039   4.773  1.00 45.80
ATOM    122  OE1 GLU    22       4.243  45.999   3.719  1.00 46.20
ATOM    123  OE2 GLU    22       3.215  45.007   5.414  1.00 46.87
ATOM    124  C   GLU    22       6.711  48.197   6.359  1.00 38.74
ATOM    125  O   GLU    22       7.482  47.954   5.423  1.00 39.26
ATOM    126  N   ASP    23       6.988  49.084   7.308  1.00 37.74
ATOM    127  CA  ASP    23       8.258  49.795   7.276  1.00 37.23
ATOM    128  CB  ASP    23       8.356  50.779   8.437  1.00 38.62
ATOM    129  CG  ASP    23       7.240  51.789   8.427  1.00 40.46
ATOM    130  OD1 ASP    23       7.104  52.508   7.408  1.00 41.26
ATOM    131  OD2 ASP    23       6.495  51.861   9.438  1.00 41.77
ATOM    132  C   ASP    23       9.371  48.760   7.382  1.00 35.54
ATOM    133  O   ASP    23      10.267  48.698   6.536  1.00 35.43
ATOM    134  N   LEU    24       9.294  47.937   8.420  1.00 33.31
ATOM    135  CA  LEU    24      10.288  46.910   8.631  1.00 32.04
ATOM    136  CB  LEU    24       9.898  46.062   9.842  1.00 31.35
ATOM    137  CG  LEU    24       9.920  46.801  11.196  1.00 31.20
ATOM    138  CD1 LEU    24       9.710  45.815  12.343  1.00 29.48
ATOM    139  CD2 LEU    24      11.253  47.526  11.367  1.00 31.51
ATOM    140  C   LEU    24      10.509  46.041   7.385  1.00 31.61
ATOM    141  O   LEU    24      11.645  45.723   7.049  1.00 31.67
ATOM    142  N   LYS    25       9.434  45.673   6.693  1.00 31.58
ATOM    143  CA  LYS    25       9.551  44.863   5.486  1.00 31.41
ATOM    144  CB  LYS    25       8.186  44.347   5.061  1.00 31.91
ATOM    145  CG  LYS    25       7.574  43.372   6.033  1.00 34.39
ATOM    146  CD  LYS    25       6.224  42.901   5.531  1.00 36.61
ATOM    147  CE  LYS    25       5.414  42.232   6.640  1.00 38.71
ATOM    148  NZ  LYS    25       3.978  42.086   6.235  1.00 39.39
ATOM    149  C   LYS    25      10.166  45.679   4.352  1.00 31.50
ATOM    150  O   LYS    25      10.969  45.170   3.568  1.00 30.92
ATOM    151  N   LYS    26       9.784  46.947   4.261  1.00 31.82
ATOM    152  CA  LYS    26      10.332  47.819   3.229  1.00 32.63
ATOM    153  CB  LYS    26       9.695  49.203   3.315  1.00 33.38
ATOM    154  CG  LYS    26      10.053  50.129   2.177  1.00 35.11
ATOM    155  CD  LYS    26       9.424  51.502   2.400  1.00 37.48
ATOM    156  CE  LYS    26       9.364  52.312   1.104  1.00 39.72
ATOM    157  NZ  LYS    26       8.706  53.645   1.307  1.00 42.62
ATOM    158  C   LYS    26      11.845  47.919   3.441  1.00 32.91
ATOM    159  O   LYS    26      12.614  48.012   2.479  1.00 32.90
ATOM    160  N   VAL    27      12.265  47.901   4.705  1.00 33.16
ATOM    161  CA  VAL    27      13.687  47.956   5.046  1.00 33.43
ATOM    162  CB  VAL    27      13.903  48.281   6.555  1.00 32.58
ATOM    163  CG1 VAL    27      15.335  47.960   6.963  1.00 32.13
ATOM    164  CG2 VAL    27      13.622  49.755   6.818  1.00 31.04
ATOM    165  C   VAL    27      14.305  46.586   4.727  1.00 33.90
ATOM    166  O   VAL    27      15.323  46.482   4.036  1.00 33.83
ATOM    167  N   MSE    28      13.668  45.536   5.223  1.00 34.26
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FIG. 4C

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ATOM    168  CA  MSE   28      14.140  44.193   4.983  1.00 34.84
ATOM    169  CB  MSE   28      13.072  43.198   5.393  1.00 35.83
ATOM    170  CG  MSE   28      13.456  41.784   5.144  1.00 38.88
ATOM    171  SE  MSE   28      12.108  40.670   5.608  1.00 45.40
ATOM    172  CE  MSE   28      11.054  40.713   4.095  1.00 42.96
ATOM    173  C   MSE   28      14.465  44.016   3.505  1.00 35.32
ATOM    174  O   MSE   28      15.571  43.621   3.144  1.00 35.22
ATOM    175  N   ARG   29      13.495  44.331   2.655  1.00 36.22
ATOM    176  CA  ARG   29      13.665  44.191   1.218  1.00 36.59
ATOM    177  CB  ARG   29      12.352  44.520   0.509  1.00 37.37
ATOM    178  CG  ARG   29      11.223  43.542   0.827  1.00 38.96
ATOM    179  CD  ARG   29       9.913  43.960   0.152  1.00 40.89
ATOM    180  NE  ARG   29       8.760  43.281   0.744  1.00 42.88
ATOM    181  CZ  ARG   29       7.621  43.889   1.081  1.00 43.80
ATOM    182  NH1 ARG   29       7.475  45.201   0.881  1.00 43.07
ATOM    183  NH2 ARG   29       6.631  43.188   1.636  1.00 44.12
ATOM    184  C   ARG   29      14.814  45.008   0.625  1.00 36.30
ATOM    185  O   ARG   29      15.615  44.469  -0.133  1.00 35.58
ATOM    186  N   ARG   30      14.906  46.296   0.948  1.00 36.85
ATOM    187  CA  ARG   30      16.008  47.091   0.410  1.00 38.41
ATOM    188  CB  ARG   30      15.944  48.543   0.894  1.00 39.31
ATOM    189  CG  ARG   30      14.676  49.285   0.513  1.00 41.96
ATOM    190  CD  ARG   30      14.742  50.763   0.933  1.00 44.07
ATOM    191  NE  ARG   30      13.415  51.384   0.995  1.00 45.48
ATOM    192  CZ  ARG   30      13.179  52.628   1.416  1.00 45.93
ATOM    193  NH1 ARG   30      14.175  53.403   1.810  1.00 45.92
ATOM    194  NH2 ARG   30      11.937  53.091   1.467  1.00 45.68
ATOM    195  C   ARG   30      17.338  46.461   0.843  1.00 39.05
ATOM    196  O   ARG   30      18.286  46.404   0.061  1.00 38.99
ATOM    197  N   MSE   31      17.408  45.999   2.092  1.00 39.11
ATOM    198  CA  MSE   31      18.615  45.348   2.596  1.00 38.96
ATOM    199  CB  MSE   31      18.374  44.784   4.002  1.00 40.43
ATOM    200  CG  MSE   31      19.512  43.922   4.599  1.00 42.62
ATOM    201  SE  MSE   31      21.083  44.819   5.027  1.00 48.46
ATOM    202  CE  MSE   31      20.438  45.988   6.389  1.00 45.46
ATOM    203  C   MSE   31      18.901  44.209   1.633  1.00 38.25
ATOM    204  O   MSE   31      19.973  44.132   1.038  1.00 38.18
ATOM    205  N   GLN   32      17.915  43.334   1.478  1.00 37.93
ATOM    206  CA  GLN   32      18.037  42.199   0.589  1.00 37.33
ATOM    207  CB  GLN   32      16.708  41.475   0.480  1.00 36.41
ATOM    208  CG  GLN   32      16.219  40.905   1.780  1.00 37.04
ATOM    209  CD  GLN   32      15.304  39.723   1.561  1.00 37.28
ATOM    210  OE1 GLN   32      15.740  38.682   1.072  1.00 38.23
ATOM    211  NE2 GLN   32      14.027  39.874   1.912  1.00 37.39
ATOM    212  C   GLN   32      18.475  42.641  -0.791  1.00 37.81
ATOM    213  O   GLN   32      19.215  41.929  -1.466  1.00 37.79
ATOM    214  N   LYS   33      18.019  43.819  -1.205  1.00 38.80
ATOM    215  CA  LYS   33      18.362  44.345  -2.516  1.00 39.85
ATOM    216  CB  LYS   33      17.525  45.588  -2.830  1.00 40.63
ATOM    217  CG  LYS   33      17.591  45.992  -4.298  1.00 42.21
ATOM    218  CD  LYS   33      16.924  47.336  -4.561  1.00 43.78
ATOM    219  CE  LYS   33      17.160  47.803  -6.006  1.00 44.42
ATOM    220  NZ  LYS   33      16.639  49.187  -6.256  1.00 44.23
ATOM    221  C   LYS   33      19.843  44.695  -2.574  1.00 40.37
ATOM    222  O   LYS   33      20.519  44.411  -3.564  1.00 40.53
ATOM    223  N   GLU   34      20.331  45.312  -1.500  1.00 40.59
ATOM    224  CA  GLU   34      21.730  45.712  -1.378  1.00 40.95
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FIG. 4D

```
ATOM    225  CB  GLU    34      21.912  46.641  -0.179  1.00 41.24
ATOM    226  CG  GLU    34      21.229  47.956  -0.359  1.00 41.42
ATOM    227  CD  GLU    34      21.476  48.506  -1.741  1.00 42.21
ATOM    228  OE1 GLU    34      22.650  48.810  -2.063  1.00 42.30
ATOM    229  OE2 GLU    34      20.493  48.613  -2.507  1.00 43.29
ATOM    230  C   GLU    34      22.667  44.528  -1.221  1.00 40.87
ATOM    231  O   GLU    34      23.770  44.527  -1.767  1.00 41.06
ATOM    232  N   MSE    35      22.233  43.534  -0.456  1.00 41.15
ATOM    233  CA  MSE    35      23.038  42.350  -0.232  1.00 41.36
ATOM    234  CB  MSE    35      22.289  41.354   0.648  1.00 41.62
ATOM    235  CG  MSE    35      22.320  41.711   2.117  1.00 43.28
ATOM    236  SE  MSE    35      21.428  40.506   3.120  1.00 46.51
ATOM    237  CE  MSE    35      22.217  38.947   2.587  1.00 45.63
ATOM    238  C   MSE    35      23.376  41.701  -1.554  1.00 41.91
ATOM    239  O   MSE    35      24.532  41.367  -1.824  1.00 42.73
ATOM    240  N   ASP    36      22.367  41.533  -2.395  1.00 42.15
ATOM    241  CA  ASP    36      22.593  40.898  -3.675  1.00 41.96
ATOM    242  CB  ASP    36      21.264  40.633  -4.369  1.00 43.56
ATOM    243  CG  ASP    36      21.446  39.947  -5.699  1.00 45.91
ATOM    244  OD1 ASP    36      21.821  40.652  -6.675  1.00 46.71
ATOM    245  OD2 ASP    36      21.232  38.707  -5.754  1.00 46.76
ATOM    246  C   ASP    36      23.502  41.717  -4.578  1.00 41.03
ATOM    247  O   ASP    36      24.406  41.178  -5.217  1.00 40.61
ATOM    248  N   ARG    37      23.257  43.021  -4.620  1.00 40.36
ATOM    249  CA  ARG    37      24.034  43.937  -5.446  1.00 39.76
ATOM    250  CB  ARG    37      23.498  45.355  -5.283  1.00 39.56
ATOM    251  CG  ARG    37      22.252  45.621  -6.112  1.00 40.04
ATOM    252  CD  ARG    37      21.465  46.815  -5.590  1.00 41.19
ATOM    253  NE  ARG    37      22.278  48.002  -5.307  1.00 41.70
ATOM    254  CZ  ARG    37      22.938  48.711  -6.221  1.00 42.38
ATOM    255  NH1 ARG    37      22.899  48.362  -7.505  1.00 42.59
ATOM    256  NH2 ARG    37      23.615  49.792  -5.851  1.00 41.94
ATOM    257  C   ARG    37      25.524  43.908  -5.152  1.00 39.94
ATOM    258  O   ARG    37      26.335  43.732  -6.059  1.00 40.39
ATOM    259  N   GLY    38      25.893  44.076  -3.890  1.00 39.94
ATOM    260  CA  GLY    38      27.305  44.063  -3.557  1.00 39.60
ATOM    261  C   GLY    38      27.933  42.689  -3.699  1.00 39.23
ATOM    262  O   GLY    38      29.163  42.546  -3.695  1.00 39.59
ATOM    263  N   LEU    39      27.087  41.677  -3.834  1.00 38.16
ATOM    264  CA  LEU    39      27.545  40.307  -3.960  1.00 37.65
ATOM    265  CB  LEU    39      26.428  39.376  -3.495  1.00 35.76
ATOM    266  CG  LEU    39      26.821  38.029  -2.900  1.00 34.52
ATOM    267  CD1 LEU    39      27.899  38.248  -1.857  1.00 33.52
ATOM    268  CD2 LEU    39      25.606  37.348  -2.284  1.00 32.44
ATOM    269  C   LEU    39      27.931  39.989  -5.407  1.00 39.20
ATOM    270  O   LEU    39      28.594  38.980  -5.681  1.00 39.88
ATOM    271  N   ARG    40      27.537  40.866  -6.329  1.00 40.51
ATOM    272  CA  ARG    40      27.809  40.656  -7.751  1.00 41.77
ATOM    273  CB  ARG    40      26.494  40.686  -8.526  1.00 42.80
ATOM    274  CG  ARG    40      25.735  39.392  -8.377  1.00 44.75
ATOM    275  CD  ARG    40      24.257  39.551  -8.636  1.00 46.47
ATOM    276  NE  ARG    40      23.639  38.239  -8.797  1.00 48.71
ATOM    277  CZ  ARG    40      22.331  38.034  -8.890  1.00 50.01
ATOM    278  NH1 ARG    40      21.497  39.064  -8.831  1.00 51.43
ATOM    279  NH2 ARG    40      21.861  36.804  -9.060  1.00 50.46
ATOM    280  C   ARG    40      28.802  41.623  -8.374  1.00 42.16
ATOM    281  O   ARG    40      28.783  42.819  -8.097  1.00 42.42
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FIG. 4E

```
ATOM    282  N   LEU  41      29.650  41.087  -9.247  1.00 42.03
ATOM    283  CA  LEU  41      30.689  41.864  -9.902  1.00 42.00
ATOM    284  CB  LEU  41      31.307  41.044 -11.041  1.00 42.00
ATOM    285  CG  LEU  41      32.577  41.650 -11.660  1.00 41.78
ATOM    286  CD1 LEU  41      33.638  41.836 -10.583  1.00 40.20
ATOM    287  CD2 LEU  41      33.087  40.747 -12.773  1.00 41.95
ATOM    288  C   LEU  41      30.278  43.237 -10.428  1.00 42.57
ATOM    289  O   LEU  41      30.920  44.243 -10.110  1.00 42.64
ATOM    290  N   GLU  42      29.219  43.292 -11.227  1.00 43.03
ATOM    291  CA  GLU  42      28.788  44.562 -11.803  1.00 44.63
ATOM    292  CB  GLU  42      27.494  44.369 -12.607  1.00 43.97
ATOM    293  CG  GLU  42      26.436  43.533 -11.922  1.00 44.02
ATOM    294  CD  GLU  42      26.546  42.057 -12.248  1.00 43.71
ATOM    295  OE1 GLU  42      27.673  41.527 -12.245  1.00 45.13
ATOM    296  OE2 GLU  42      25.504  41.416 -12.496  1.00 43.50
ATOM    297  C   GLU  42      28.616  45.714 -10.805  1.00 46.21
ATOM    298  O   GLU  42      28.963  46.860 -11.103  1.00 46.22
ATOM    299  N   THR  43      28.105  45.413  -9.616  1.00 47.90
ATOM    300  CA  THR  43      27.873  46.443  -8.608  1.00 49.10
ATOM    301  CB  THR  43      26.370  46.533  -8.285  1.00 48.63
ATOM    302  OG1 THR  43      25.772  45.242  -8.465  1.00 47.66
ATOM    303  CG2 THR  43      25.679  47.531  -9.192  1.00 48.90
ATOM    304  C   THR  43      28.629  46.226  -7.302  1.00 50.94
ATOM    305  O   THR  43      28.481  47.008  -6.362  1.00 51.52
ATOM    306  N   HIS  44      29.456  45.185  -7.249  1.00 52.58
ATOM    307  CA  HIS  44      30.204  44.854  -6.037  1.00 53.89
ATOM    308  CB  HIS  44      31.210  43.727  -6.311  1.00 54.68
ATOM    309  CG  HIS  44      32.552  44.208  -6.775  1.00 55.77
ATOM    310  CD2 HIS  44      33.748  44.257  -6.139  1.00 55.82
ATOM    311  ND1 HIS  44      32.758  44.772  -8.017  1.00 56.36
ATOM    312  CE1 HIS  44      34.020  45.146  -8.125  1.00 56.30
ATOM    313  NE2 HIS  44      34.643  44.845  -6.999  1.00 56.06
ATOM    314  C   HIS  44      30.950  46.013  -5.398  1.00 54.87
ATOM    315  O   HIS  44      30.823  46.254  -4.199  1.00 55.06
ATOM    316  N   GLU  45      31.724  46.732  -6.203  1.00 56.25
ATOM    317  CA  GLU  45      32.540  47.826  -5.703  1.00 57.17
ATOM    318  CB  GLU  45      33.618  48.180  -6.721  1.00 59.35
ATOM    319  CG  GLU  45      33.146  49.127  -7.800  1.00 61.61
ATOM    320  CD  GLU  45      34.107  50.279  -7.985  1.00 63.07
ATOM    321  OE1 GLU  45      35.228  50.038  -8.487  1.00 63.72
ATOM    322  OE2 GLU  45      33.747  51.420  -7.613  1.00 64.00
ATOM    323  C   GLU  45      31.762  49.074  -5.356  1.00 56.66
ATOM    324  O   GLU  45      32.295  49.985  -4.732  1.00 56.54
ATOM    325  N   GLU  46      30.508  49.135  -5.772  1.00 56.24
ATOM    326  CA  GLU  46      29.708  50.306  -5.456  1.00 56.37
ATOM    327  CB  GLU  46      29.542  51.157  -6.704  1.00 57.92
ATOM    328  CG  GLU  46      30.881  51.645  -7.212  1.00 60.77
ATOM    329  CD  GLU  46      30.782  52.400  -8.515  1.00 62.28
ATOM    330  OE1 GLU  46      30.566  51.762  -9.571  1.00 62.25
ATOM    331  OE2 GLU  46      30.914  53.641  -8.474  1.00 63.95
ATOM    332  C   GLU  46      28.366  49.891  -4.873  1.00 55.40
ATOM    333  O   GLU  46      27.309  50.123  -5.457  1.00 55.75
ATOM    334  N   ALA  47      28.440  49.264  -3.704  1.00 53.89
ATOM    335  CA  ALA  47      27.273  48.783  -2.987  1.00 51.80
ATOM    336  CB  ALA  47      27.140  47.280  -3.159  1.00 52.36
ATOM    337  C   ALA  47      27.470  49.111  -1.524  1.00 49.98
ATOM    338  O   ALA  47      28.448  48.664  -0.923  1.00 50.36
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FIG. 4F

```
ATOM    339  N   SER  48      26.553  49.894  -0.960  1.00 47.18
ATOM    340  CA  SER  48      26.630  50.267   0.444  1.00 44.70
ATOM    341  CB  SER  48      25.299  50.860   0.897  1.00 46.13
ATOM    342  OG  SER  48      24.243  49.927   0.720  1.00 47.87
ATOM    343  C   SER  48      26.965  49.041   1.287  1.00 42.45
ATOM    344  O   SER  48      27.841  49.082   2.147  1.00 42.01
ATOM    345  N   VAL  49      26.261  47.946   1.037  1.00 40.48
ATOM    346  CA  VAL  49      26.516  46.713   1.762  1.00 38.96
ATOM    347  CB  VAL  49      25.231  45.849   1.875  1.00 38.62
ATOM    348  CG1 VAL  49      25.496  44.625   2.740  1.00 38.40
ATOM    349  CG2 VAL  49      24.102  46.672   2.472  1.00 37.16
ATOM    350  C   VAL  49      27.572  45.997   0.929  1.00 37.97
ATOM    351  O   VAL  49      27.266  45.474  -0.137  1.00 38.42
ATOM    352  N   LYS  50      28.810  45.982   1.422  1.00 36.51
ATOM    353  CA  LYS  50      29.937  45.385   0.703  1.00 34.95
ATOM    354  CB  LYS  50      31.250  45.843   1.334  1.00 35.51
ATOM    355  CG  LYS  50      31.574  47.322   1.091  1.00 36.68
ATOM    356  CD  LYS  50      30.676  48.249   1.913  1.00 39.05
ATOM    357  CE  LYS  50      30.865  48.018   3.419  1.00 39.54
ATOM    358  NZ  LYS  50      32.316  48.157   3.792  1.00 40.04
ATOM    359  C   LYS  50      30.012  43.879   0.482  1.00 33.72
ATOM    360  O   LYS  50      30.845  43.421  -0.293  1.00 33.30
ATOM    361  N   MSE  51      29.171  43.100   1.147  1.00 33.02
ATOM    362  CA  MSE  51      29.209  41.647   0.967  1.00 32.08
ATOM    363  CB  MSE  51      28.291  41.257  -0.190  1.00 34.01
ATOM    364  CG  MSE  51      26.867  41.744  -0.025  1.00 36.03
ATOM    365  SE  MSE  51      26.148  41.146   1.529  1.00 40.73
ATOM    366  CE  MSE  51      25.558  39.411   1.085  1.00 37.98
ATOM    367  C   MSE  51      30.637  41.180   0.666  1.00 30.17
ATOM    368  O   MSE  51      30.928  40.723  -0.437  1.00 30.22
ATOM    369  N   LEU  52      31.518  41.295   1.650  1.00 28.96
ATOM    370  CA  LEU  52      32.920  40.928   1.487  1.00 27.43
ATOM    371  CB  LEU  52      33.769  41.839   2.357  1.00 28.05
ATOM    372  CG  LEU  52      33.649  43.319   1.991  1.00 28.52
ATOM    373  CD1 LEU  52      34.222  44.171   3.116  1.00 28.77
ATOM    374  CD2 LEU  52      34.369  43.583   0.658  1.00 28.75
ATOM    375  C   LEU  52      33.273  39.482   1.803  1.00 26.61
ATOM    376  O   LEU  52      32.997  38.995   2.893  1.00 25.26
ATOM    377  N   PRO  53      33.911  38.774   0.844  1.00 27.04
ATOM    378  CD  PRO  53      34.270  39.142  -0.540  1.00 25.69
ATOM    379  CA  PRO  53      34.264  37.375   1.133  1.00 27.99
ATOM    380  CB  PRO  53      34.807  36.864  -0.204  1.00 26.92
ATOM    381  CG  PRO  53      34.184  37.825  -1.241  1.00 25.77
ATOM    382  C   PRO  53      35.314  37.361   2.239  1.00 28.40
ATOM    383  O   PRO  53      36.152  38.271   2.317  1.00 28.36
ATOM    384  N   THR  54      35.255  36.329   3.080  1.00 29.46
ATOM    385  CA  THR  54      36.149  36.142   4.226  1.00 30.53
ATOM    386  CB  THR  54      35.317  35.951   5.502  1.00 29.48
ATOM    387  OG1 THR  54      34.589  34.711   5.418  1.00 27.97
ATOM    388  CG2 THR  54      34.324  37.084   5.659  1.00 29.42
ATOM    389  C   THR  54      37.018  34.884   4.071  1.00 31.60
ATOM    390  O   THR  54      37.657  34.423   5.025  1.00 32.25
ATOM    391  N   TYR  55      37.017  34.311   2.877  1.00 32.63
ATOM    392  CA  TYR  55      37.763  33.089   2.615  1.00 34.41
ATOM    393  CB  TYR  55      39.249  33.421   2.405  1.00 33.07
ATOM    394  CG  TYR  55      39.458  34.175   1.101  1.00 32.58
ATOM    395  CD1 TYR  55      39.518  35.571   1.067  1.00 32.44
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FIG. 4G

ATOM	396	CE1	TYR	55	39.572	36.263	-0.157	1.00	32.48
ATOM	397	CD2	TYR	55	39.467	33.492	-0.117	1.00	31.97
ATOM	398	CE2	TYR	55	39.516	34.172	-1.335	1.00	31.83
ATOM	399	CZ	TYR	55	39.566	35.548	-1.351	1.00	32.18
ATOM	400	OH	TYR	55	39.575	36.200	-2.568	1.00	32.67
ATOM	401	C	TYR	55	37.559	31.956	3.637	1.00	36.06
ATOM	402	O	TYR	55	38.314	30.991	3.665	1.00	37.61
ATOM	403	N	VAL	56	36.518	32.059	4.459	1.00	38.03
ATOM	404	CA	VAL	56	36.199	31.006	5.429	1.00	39.87
ATOM	405	CB	VAL	56	35.483	31.586	6.663	1.00	38.75
ATOM	406	CG1	VAL	56	35.202	30.492	7.669	1.00	38.10
ATOM	407	CG2	VAL	56	36.336	32.660	7.285	1.00	38.76
ATOM	408	C	VAL	56	35.249	30.032	4.706	1.00	42.20
ATOM	409	O	VAL	56	34.098	30.376	4.418	1.00	42.02
ATOM	410	N	ARG	57	35.718	28.821	4.414	1.00	44.49
ATOM	411	CA	ARG	57	34.896	27.860	3.676	1.00	47.07
ATOM	412	CB	ARG	57	35.688	27.288	2.499	1.00	48.02
ATOM	413	CG	ARG	57	36.209	28.310	1.508	1.00	49.08
ATOM	414	CD	ARG	57	36.558	27.626	0.185	1.00	49.69
ATOM	415	NE	ARG	57	37.239	28.528	-0.737	1.00	49.50
ATOM	416	CZ	ARG	57	38.367	29.167	-0.447	1.00	48.83
ATOM	417	NH1	ARG	57	38.938	28.997	0.745	1.00	48.13
ATOM	418	NH2	ARG	57	38.915	29.978	-1.345	1.00	47.51
ATOM	419	C	ARG	57	34.311	26.695	4.449	1.00	48.57
ATOM	420	O	ARG	57	34.810	26.310	5.500	1.00	48.65
ATOM	421	N	SER	58	33.256	26.117	3.891	1.00	51.15
ATOM	422	CA	SER	58	32.589	24.973	4.501	1.00	54.78
ATOM	423	CB	SER	58	31.204	24.793	3.882	1.00	54.26
ATOM	424	OG	SER	58	31.258	24.980	2.475	1.00	54.39
ATOM	425	C	SER	58	33.419	23.708	4.295	1.00	57.39
ATOM	426	O	SER	58	33.097	22.645	4.823	1.00	57.47
ATOM	427	N	THR	59	34.484	23.840	3.510	1.00	60.71
ATOM	428	CA	THR	59	35.392	22.740	3.216	1.00	64.02
ATOM	429	CB	THR	59	35.886	22.823	1.758	1.00	63.73
ATOM	430	OG1	THR	59	36.637	24.029	1.570	1.00	63.22
ATOM	431	CG2	THR	59	34.704	22.843	0.801	1.00	63.87
ATOM	432	C	THR	59	36.571	22.880	4.176	1.00	67.10
ATOM	433	O	THR	59	37.554	23.562	3.884	1.00	67.44
ATOM	434	N	PRO	60	36.480	22.238	5.349	1.00	69.75
ATOM	435	CD	PRO	60	35.366	21.412	5.854	1.00	70.63
ATOM	436	CA	PRO	60	37.556	22.320	6.337	1.00	71.72
ATOM	437	CB	PRO	60	36.841	21.982	7.636	1.00	71.72
ATOM	438	CG	PRO	60	35.909	20.881	7.182	1.00	71.50
ATOM	439	C	PRO	60	38.709	21.370	6.056	1.00	73.48
ATOM	440	O	PRO	60	39.522	21.609	5.158	1.00	73.53
ATOM	441	N	GLU	61	38.754	20.287	6.830	1.00	75.48
ATOM	442	CA	GLU	61	39.808	19.283	6.731	1.00	76.98
ATOM	443	CB	GLU	61	39.969	18.788	5.289	1.00	78.43
ATOM	444	CG	GLU	61	40.806	17.516	5.161	1.00	80.68
ATOM	445	CD	GLU	61	42.177	17.744	4.530	1.00	81.88
ATOM	446	OE1	GLU	61	42.993	18.498	5.100	1.00	82.28
ATOM	447	OE2	GLU	61	42.442	17.156	3.458	1.00	82.68
ATOM	448	C	GLU	61	41.083	19.969	7.194	1.00	77.00
ATOM	449	O	GLU	61	41.942	20.327	6.389	1.00	77.10
ATOM	450	N	GLY	62	41.177	20.181	8.502	1.00	76.85
ATOM	451	CA	GLY	62	42.344	20.826	9.069	1.00	76.72
ATOM	452	C	GLY	62	42.415	20.539	10.555	1.00	76.65

FIG. 4H

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ATOM    453  O   GLY   62      42.507  19.380  10.969  1.00 76.79
ATOM    454  N   SER   63      42.361  21.594  11.362  1.00 76.25
ATOM    455  CA  SER   63      42.417  21.458  12.814  1.00 75.06
ATOM    456  CB  SER   63      41.401  20.413  13.300  1.00 75.92
ATOM    457  OG  SER   63      41.350  20.363  14.718  1.00 76.69
ATOM    458  C   SER   63      43.818  21.062  13.259  1.00 73.60
ATOM    459  O   SER   63      44.090  19.899  13.561  1.00 73.10
ATOM    460  N   GLU   64      44.705  22.045  13.280  1.00 71.83
ATOM    461  CA  GLU   64      46.071  21.819  13.703  1.00 70.12
ATOM    462  CB  GLU   64      46.996  22.824  13.011  1.00 71.42
ATOM    463  CG  GLU   64      48.464  22.726  13.417  1.00 73.74
ATOM    464  CD  GLU   64      49.014  21.309  13.342  1.00 74.84
ATOM    465  OE1 GLU   64      48.623  20.466  14.187  1.00 75.26
ATOM    466  OE2 GLU   64      49.837  21.041  12.434  1.00 75.45
ATOM    467  C   GLU   64      46.136  21.971  15.221  1.00 67.97
ATOM    468  O   GLU   64      46.775  22.886  15.734  1.00 68.33
ATOM    469  N   VAL   65      45.448  21.076  15.927  1.00 65.13
ATOM    470  CA  VAL   65      45.400  21.067  17.391  1.00 62.32
ATOM    471  CB  VAL   65      45.335  19.621  17.918  1.00 62.48
ATOM    472  CG1 VAL   65      45.487  19.607  19.430  1.00 62.45
ATOM    473  CG2 VAL   65      44.011  18.975  17.508  1.00 62.79
ATOM    474  C   VAL   65      46.587  21.752  18.055  1.00 60.42
ATOM    475  O   VAL   65      47.703  21.708  17.540  1.00 60.54
ATOM    476  N   GLY   66      46.354  22.386  19.200  1.00 58.26
ATOM    477  CA  GLY   66      47.454  23.043  19.888  1.00 55.67
ATOM    478  C   GLY   66      47.081  24.174  20.823  1.00 53.42
ATOM    479  O   GLY   66      46.153  24.052  21.615  1.00 54.08
ATOM    480  N   ASP   67      47.832  25.267  20.739  1.00 51.06
ATOM    481  CA  ASP   67      47.614  26.460  21.549  1.00 48.67
ATOM    482  CB  ASP   67      48.617  26.531  22.703  1.00 49.14
ATOM    483  CG  ASP   67      48.381  25.462  23.751  1.00 49.34
ATOM    484  OD1 ASP   67      48.201  24.287  23.365  1.00 49.37
ATOM    485  OD2 ASP   67      48.386  25.791  24.956  1.00 49.62
ATOM    486  C   ASP   67      47.832  27.634  20.612  1.00 47.26
ATOM    487  O   ASP   67      48.786  27.635  19.827  1.00 47.44
ATOM    488  N   PHE   68      46.955  28.632  20.678  1.00 45.41
ATOM    489  CA  PHE   68      47.075  29.778  19.785  1.00 43.60
ATOM    490  CB  PHE   68      46.031  29.682  18.667  1.00 41.17
ATOM    491  CG  PHE   68      46.032  28.361  17.946  1.00 39.29
ATOM    492  CD1 PHE   68      45.621  27.199  18.592  1.00 38.55
ATOM    493  CD2 PHE   68      46.468  28.272  16.623  1.00 38.76
ATOM    494  CE1 PHE   68      45.647  25.966  17.934  1.00 38.24
ATOM    495  CE2 PHE   68      46.498  27.050  15.959  1.00 37.31
ATOM    496  CZ  PHE   68      46.086  25.893  16.619  1.00 37.76
ATOM    497  C   PHE   68      46.918  31.096  20.514  1.00 43.33
ATOM    498  O   PHE   68      46.395  31.147  21.621  1.00 43.27
ATOM    499  N   LEU   69      47.386  32.166  19.889  1.00 43.51
ATOM    500  CA  LEU   69      47.274  33.475  20.497  1.00 44.73
ATOM    501  CB  LEU   69      48.625  34.197  20.518  1.00 45.26
ATOM    502  CG  LEU   69      48.781  34.949  21.848  1.00 46.33
ATOM    503  CD1 LEU   69      49.166  33.928  22.932  1.00 46.09
ATOM    504  CD2 LEU   69      49.811  36.072  21.748  1.00 45.48
ATOM    505  C   LEU   69      46.275  34.278  19.681  1.00 45.37
ATOM    506  O   LEU   69      46.448  34.451  18.470  1.00 45.62
ATOM    507  N   SER   70      45.228  34.758  20.351  1.00 45.75
ATOM    508  CA  SER   70      44.177  35.528  19.697  1.00 44.98
ATOM    509  CB  SER   70      42.794  34.984  20.074  1.00 44.61
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FIG. 4I

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ATOM    510  OG  SER   70      42.697  33.589  19.844  1.00 44.25
ATOM    511  C   SER   70      44.250  36.978  20.109  1.00 44.92
ATOM    512  O   SER   70      44.451  37.289  21.277  1.00 44.67
ATOM    513  N   LEU   71      44.095  37.858  19.130  1.00 45.85
ATOM    514  CA  LEU   71      44.092  39.294  19.366  1.00 47.27
ATOM    515  CB  LEU   71      45.064  40.000  18.421  1.00 47.71
ATOM    516  CG  LEU   71      46.552  39.942  18.787  1.00 49.06
ATOM    517  CD1 LEU   71      47.008  38.497  19.039  1.00 49.69
ATOM    518  CD2 LEU   71      47.348  40.572  17.656  1.00 49.35
ATOM    519  C   LEU   71      42.668  39.752  19.082  1.00 47.94
ATOM    520  O   LEU   71      41.873  38.997  18.499  1.00 48.06
ATOM    521  N   ASP   72      42.333  40.976  19.479  1.00 48.20
ATOM    522  CA  ASP   72      40.985  41.451  19.244  1.00 48.67
ATOM    523  CB  ASP   72      40.043  40.807  20.262  1.00 48.71
ATOM    524  CG  ASP   72      38.668  41.420  20.243  1.00 49.13
ATOM    525  OD1 ASP   72      38.090  41.549  19.144  1.00 49.57
ATOM    526  OD2 ASP   72      38.168  41.777  21.331  1.00 50.11
ATOM    527  C   ASP   72      40.819  42.962  19.258  1.00 48.98
ATOM    528  O   ASP   72      40.247  43.530  20.187  1.00 48.82
ATOM    529  N   LEU   73      41.312  43.613  18.214  1.00 49.73
ATOM    530  CA  LEU   73      41.193  45.060  18.117  1.00 51.48
ATOM    531  CB  LEU   73      42.199  45.603  17.096  1.00 50.80
ATOM    532  CG  LEU   73      42.160  47.096  16.774  1.00 50.07
ATOM    533  CD1 LEU   73      42.358  47.902  18.045  1.00 50.10
ATOM    534  CD2 LEU   73      43.223  47.421  15.738  1.00 49.97
ATOM    535  C   LEU   73      39.764  45.392  17.687  1.00 52.93
ATOM    536  O   LEU   73      38.909  44.507  17.628  1.00 52.38
ATOM    537  N   GLY   74      39.504  46.665  17.401  1.00 54.88
ATOM    538  CA  GLY   74      38.177  47.068  16.983  1.00 56.88
ATOM    539  C   GLY   74      37.285  47.420  18.148  1.00 58.48
ATOM    540  O   GLY   74      36.476  48.348  18.071  1.00 58.31
ATOM    541  N   GLY   75      37.428  46.668  19.233  1.00 60.27
ATOM    542  CA  GLY   75      36.621  46.925  20.410  1.00 62.46
ATOM    543  C   GLY   75      37.020  48.230  21.074  1.00 63.75
ATOM    544  O   GLY   75      37.824  49.005  20.536  1.00 64.06
ATOM    545  N   THR   76      36.452  48.481  22.248  1.00 64.50
ATOM    546  CA  THR   76      36.759  49.697  22.991  1.00 65.42
ATOM    547  CB  THR   76      35.905  49.776  24.266  1.00 66.28
ATOM    548  OG1 THR   76      36.361  48.791  25.203  1.00 67.43
ATOM    549  CG2 THR   76      34.425  49.505  23.938  1.00 66.14
ATOM    550  C   THR   76      38.238  49.651  23.385  1.00 65.25
ATOM    551  O   THR   76      39.005  50.595  23.152  1.00 65.01
ATOM    552  N   ASN   77      38.622  48.528  23.980  1.00 64.74
ATOM    553  CA  ASN   77      39.987  48.309  24.412  1.00 64.17
ATOM    554  CB  ASN   77      40.015  47.966  25.903  1.00 65.44
ATOM    555  CG  ASN   77      39.346  49.027  26.765  1.00 66.47
ATOM    556  OD1 ASN   77      39.656  50.219  26.663  1.00 67.13
ATOM    557  ND2 ASN   77      38.431  48.596  27.629  1.00 66.65
ATOM    558  C   ASN   77      40.547  47.149  23.603  1.00 63.19
ATOM    559  O   ASN   77      39.795  46.303  23.120  1.00 62.58
ATOM    560  N   PHE   78      41.866  47.123  23.446  1.00 62.14
ATOM    561  CA  PHE   78      42.526  46.051  22.708  1.00 61.12
ATOM    562  CB  PHE   78      43.887  46.514  22.172  1.00 61.81
ATOM    563  CG  PHE   78      44.684  45.420  21.516  1.00 62.50
ATOM    564  CD1 PHE   78      44.347  44.956  20.245  1.00 62.81
ATOM    565  CD2 PHE   78      45.741  44.818  22.189  1.00 62.99
ATOM    566  CE1 PHE   78      45.051  43.899  19.655  1.00 62.72
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FIG. 4J

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ATOM    567  CE2 PHE   78      46.450  43.763  21.607  1.00 63.38
ATOM    568  CZ  PHE   78      46.103  43.301  20.336  1.00 63.01
ATOM    569  C   PHE   78      42.732  44.893  23.668  1.00 60.09
ATOM    570  O   PHE   78      43.065  45.100  24.834  1.00 60.08
ATOM    571  N   ARG   79      42.528  43.675  23.184  1.00 58.63
ATOM    572  CA  ARG   79      42.706  42.504  24.025  1.00 57.40
ATOM    573  CB  ARG   79      41.367  41.819  24.280  1.00 57.06
ATOM    574  CG  ARG   79      41.481  40.637  25.222  1.00 57.49
ATOM    575  CD  ARG   79      40.221  39.819  25.219  1.00 57.47
ATOM    576  NE  ARG   79      39.062  40.646  25.504  1.00 57.16
ATOM    577  CZ  ARG   79      37.818  40.266  25.267  1.00 57.69
ATOM    578  NH1 ARG   79      37.586  39.071  24.738  1.00 57.38
ATOM    579  NH2 ARG   79      36.812  41.080  25.555  1.00 58.45
ATOM    580  C   ARG   79      43.663  41.522  23.368  1.00 56.71
ATOM    581  O   ARG   79      43.926  41.619  22.170  1.00 57.24
ATOM    582  N   VAL   80      44.180  40.590  24.167  1.00 55.50
ATOM    583  CA  VAL   80      45.114  39.557  23.724  1.00 54.27
ATOM    584  CB  VAL   80      46.576  39.947  23.996  1.00 54.31
ATOM    585  CG1 VAL   80      47.491  38.779  23.674  1.00 54.49
ATOM    586  CG2 VAL   80      46.960  41.158  23.166  1.00 54.39
ATOM    587  C   VAL   80      44.806  38.327  24.555  1.00 54.04
ATOM    588  O   VAL   80      44.517  38.447  25.738  1.00 53.31
ATOM    589  N   MSE   81      44.881  37.144  23.957  1.00 54.52
ATOM    590  CA  MSE   81      44.568  35.935  24.703  1.00 54.59
ATOM    591  CB  MSE   81      43.053  35.804  24.828  1.00 57.08
ATOM    592  CG  MSE   81      42.300  36.025  23.520  1.00 60.39
ATOM    593  SE  MSE   81      40.534  36.437  23.792  1.00 65.62
ATOM    594  CE  MSE   81      39.999  34.926  24.679  1.00 62.03
ATOM    595  C   MSE   81      45.142  34.645  24.146  1.00 53.56
ATOM    596  O   MSE   81      45.598  34.582  23.007  1.00 52.99
ATOM    597  N   LEU   82      45.096  33.611  24.978  1.00 52.63
ATOM    598  CA  LEU   82      45.602  32.292  24.638  1.00 51.86
ATOM    599  CB  LEU   82      46.660  31.863  25.665  1.00 52.75
ATOM    600  CG  LEU   82      47.261  30.455  25.542  1.00 53.22
ATOM    601  CD1 LEU   82      48.562  30.521  24.736  1.00 52.42
ATOM    602  CD2 LEU   82      47.523  29.882  26.937  1.00 53.00
ATOM    603  C   LEU   82      44.461  31.286  24.650  1.00 51.18
ATOM    604  O   LEU   82      43.718  31.186  25.632  1.00 51.20
ATOM    605  N   VAL   83      44.333  30.535  23.563  1.00 50.58
ATOM    606  CA  VAL   83      43.292  29.522  23.448  1.00 50.00
ATOM    607  CB  VAL   83      42.274  29.887  22.362  1.00 49.63
ATOM    608  CG1 VAL   83      41.213  28.794  22.262  1.00 49.26
ATOM    609  CG2 VAL   83      41.660  31.244  22.670  1.00 48.32
ATOM    610  C   VAL   83      43.914  28.187  23.080  1.00 50.53
ATOM    611  O   VAL   83      44.759  28.122  22.192  1.00 50.93
ATOM    612  N   LYS   84      43.496  27.127  23.763  1.00 51.05
ATOM    613  CA  LYS   84      44.017  25.788  23.504  1.00 51.89
ATOM    614  CB  LYS   84      44.338  25.061  24.826  1.00 51.79
ATOM    615  CG  LYS   84      44.716  23.581  24.659  1.00 51.85
ATOM    616  CD  LYS   84      44.951  22.870  26.009  1.00 51.58
ATOM    617  CE  LYS   84      46.429  22.848  26.422  1.00 50.92
ATOM    618  NZ  LYS   84      47.041  24.198  26.592  1.00 50.33
ATOM    619  C   LYS   84      42.997  24.983  22.708  1.00 52.68
ATOM    620  O   LYS   84      42.115  24.327  23.282  1.00 53.00
ATOM    621  N   VAL   85      43.124  25.038  21.383  1.00 52.91
ATOM    622  CA  VAL   85      42.224  24.319  20.488  1.00 52.70
ATOM    623  CB  VAL   85      42.399  24.805  19.048  1.00 51.79
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FIG. 4K

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ATOM    624  CG1 VAL    85      41.302  24.232  18.176  1.00 52.19
ATOM    625  CG2 VAL    85      42.389  26.319  19.017  1.00 51.59
ATOM    626  C   VAL    85      42.525  22.823  20.548  1.00 53.51
ATOM    627  O   VAL    85      43.637  22.389  20.243  1.00 53.87
ATOM    628  N   GLY    86      41.534  22.037  20.952  1.00 54.38
ATOM    629  CA  GLY    86      41.726  20.603  21.053  1.00 55.35
ATOM    630  C   GLY    86      40.901  19.810  20.060  1.00 56.21
ATOM    631  O   GLY    86      40.136  20.370  19.278  1.00 55.63
ATOM    632  N   GLU    87      41.050  18.493  20.106  1.00 57.81
ATOM    633  CA  GLU    87      40.339  17.611  19.195  1.00 59.64
ATOM    634  CB  GLU    87      41.290  16.529  18.673  1.00 60.88
ATOM    635  CG  GLU    87      40.680  15.648  17.611  1.00 62.26
ATOM    636  CD  GLU    87      40.215  16.457  16.423  1.00 63.21
ATOM    637  OE1 GLU    87      41.072  16.931  15.644  1.00 63.20
ATOM    638  OE2 GLU    87      38.989  16.631  16.278  1.00 64.58
ATOM    639  C   GLU    87      39.133  16.959  19.859  1.00 60.12
ATOM    640  O   GLU    87      39.271  16.187  20.810  1.00 60.00
ATOM    641  N   GLY    88      37.948  17.273  19.347  1.00 60.93
ATOM    642  CA  GLY    88      36.735  16.707  19.902  1.00 61.61
ATOM    643  C   GLY    88      35.840  16.120  18.833  1.00 62.11
ATOM    644  O   GLY    88      36.038  16.346  17.638  1.00 61.67
ATOM    645  N   GLU    89      34.845  15.363  19.274  1.00 62.79
ATOM    646  CA  GLU    89      33.898  14.724  18.372  1.00 63.90
ATOM    647  CB  GLU    89      32.782  14.089  19.203  1.00 63.50
ATOM    648  CG  GLU    89      33.304  13.137  20.275  1.00 62.64
ATOM    649  CD  GLU    89      32.214  12.623  21.203  1.00 62.46
ATOM    650  OE1 GLU    89      32.510  11.728  22.019  1.00 62.39
ATOM    651  OE2 GLU    89      31.064  13.110  21.128  1.00 62.11
ATOM    652  C   GLU    89      33.312  15.688  17.325  1.00 65.16
ATOM    653  O   GLU    89      32.975  16.837  17.634  1.00 64.98
ATOM    654  N   GLU    90      33.204  15.205  16.087  1.00 66.03
ATOM    655  CA  GLU    90      32.667  15.977  14.958  1.00 66.67
ATOM    656  CB  GLU    90      31.135  15.974  14.978  1.00 67.21
ATOM    657  CG  GLU    90      30.495  14.620  14.717  1.00 66.83
ATOM    658  CD  GLU    90      28.986  14.662  14.869  1.00 67.49
ATOM    659  OE1 GLU    90      28.308  15.273  14.009  1.00 67.17
ATOM    660  OE2 GLU    90      28.480  14.090  15.858  1.00 66.84
ATOM    661  C   GLU    90      33.149  17.421  14.871  1.00 66.91
ATOM    662  O   GLU    90      32.623  18.212  14.080  1.00 66.74
ATOM    663  N   GLY    91      34.149  17.769  15.671  1.00 67.05
ATOM    664  CA  GLY    91      34.649  19.126  15.628  1.00 67.38
ATOM    665  C   GLY    91      36.036  19.339  16.201  1.00 67.42
ATOM    666  O   GLY    91      37.025  18.797  15.708  1.00 68.24
ATOM    667  N   GLN    92      36.094  20.154  17.246  1.00 66.86
ATOM    668  CA  GLN    92      37.335  20.492  17.929  1.00 65.93
ATOM    669  CB  GLN    92      38.395  20.968  16.924  1.00 66.17
ATOM    670  CG  GLN    92      38.007  22.215  16.159  1.00 66.24
ATOM    671  CD  GLN    92      38.564  22.236  14.750  1.00 66.57
ATOM    672  OE1 GLN    92      38.432  21.260  14.007  1.00 66.37
ATOM    673  NE2 GLN    92      39.177  23.356  14.367  1.00 66.54
ATOM    674  C   GLN    92      36.999  21.605  18.920  1.00 65.21
ATOM    675  O   GLN    92      36.625  22.721  18.530  1.00 65.44
ATOM    676  N   TRP    93      37.111  21.278  20.204  1.00 63.62
ATOM    677  CA  TRP    93      36.820  22.227  21.261  1.00 61.61
ATOM    678  CB  TRP    93      36.859  21.540  22.626  1.00 62.77
ATOM    679  CG  TRP    93      38.050  20.641  22.857  1.00 63.86
ATOM    680  CD2 TRP    93      39.213  20.943  23.637  1.00 64.17
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FIG. 4L

ATOM	681	CE2	TRP	93	40.026	19.787	23.645	1.00	64.21
ATOM	682	CE3	TRP	93	39.647	22.080	24.336	1.00	64.11
ATOM	683	CD1	TRP	93	38.206	19.349	22.424	1.00	63.84
ATOM	684	NE1	TRP	93	39.387	18.830	22.897	1.00	63.69
ATOM	685	CZ2	TRP	93	41.246	19.731	24.324	1.00	64.43
ATOM	686	CZ3	TRP	93	40.859	22.026	25.009	1.00	64.63
ATOM	687	CH2	TRP	93	41.645	20.857	24.999	1.00	64.71
ATOM	688	C	TRP	93	37.784	23.393	21.248	1.00	59.53
ATOM	689	O	TRP	93	38.733	23.420	20.474	1.00	59.18
ATOM	690	N	SER	94	37.521	24.366	22.106	1.00	57.94
ATOM	691	CA	SER	94	38.353	25.549	22.207	1.00	56.46
ATOM	692	CB	SER	94	37.880	26.615	21.219	1.00	56.58
ATOM	693	OG	SER	94	36.504	26.899	21.412	1.00	56.78
ATOM	694	C	SER	94	38.185	26.050	23.624	1.00	55.56
ATOM	695	O	SER	94	37.142	25.822	24.237	1.00	55.36
ATOM	696	N	VAL	95	39.208	26.722	24.146	1.00	54.53
ATOM	697	CA	VAL	95	39.152	27.248	25.504	1.00	53.17
ATOM	698	CB	VAL	95	39.511	26.183	26.549	1.00	52.17
ATOM	699	CG1	VAL	95	39.742	26.844	27.891	1.00	52.13
ATOM	700	CG2	VAL	95	38.396	25.172	26.666	1.00	51.73
ATOM	701	C	VAL	95	40.099	28.399	25.719	1.00	52.74
ATOM	702	O	VAL	95	41.268	28.315	25.357	1.00	53.14
ATOM	703	N	LYS	96	39.587	29.469	26.318	1.00	52.63
ATOM	704	CA	LYS	96	40.402	30.637	26.629	1.00	52.93
ATOM	705	CB	LYS	96	39.513	31.849	26.932	1.00	53.25
ATOM	706	CG	LYS	96	40.277	33.129	27.231	1.00	53.79
ATOM	707	CD	LYS	96	39.910	33.706	28.595	1.00	54.80
ATOM	708	CE	LYS	96	38.427	34.102	28.682	1.00	55.69
ATOM	709	NZ	LYS	96	38.027	35.162	27.696	1.00	55.59
ATOM	710	C	LYS	96	41.154	30.218	27.882	1.00	52.96
ATOM	711	O	LYS	96	40.546	29.733	28.834	1.00	52.93
ATOM	712	N	THR	97	42.470	30.384	27.886	1.00	53.38
ATOM	713	CA	THR	97	43.253	29.980	29.050	1.00	53.93
ATOM	714	CB	THR	97	44.238	28.850	28.684	1.00	53.99
ATOM	715	OG1	THR	97	43.512	27.736	28.151	1.00	52.99
ATOM	716	CG2	THR	97	44.998	28.394	29.918	1.00	55.29
ATOM	717	C	THR	97	44.036	31.132	29.670	1.00	53.82
ATOM	718	O	THR	97	44.330	31.123	30.866	1.00	53.34
ATOM	719	N	LYS	98	44.373	32.117	28.848	1.00	53.85
ATOM	720	CA	LYS	98	45.115	33.276	29.315	1.00	54.60
ATOM	721	CB	LYS	98	46.627	33.096	29.087	1.00	55.51
ATOM	722	CG	LYS	98	47.220	31.809	29.652	1.00	56.78
ATOM	723	CD	LYS	98	47.074	31.733	31.162	1.00	58.23
ATOM	724	CE	LYS	98	47.553	30.389	31.713	1.00	58.82
ATOM	725	NZ	LYS	98	47.404	30.320	33.201	1.00	58.98
ATOM	726	C	LYS	98	44.644	34.479	28.518	1.00	54.54
ATOM	727	O	LYS	98	44.323	34.360	27.329	1.00	54.79
ATOM	728	N	HIS	99	44.590	35.632	29.173	1.00	54.03
ATOM	729	CA	HIS	99	44.193	36.853	28.496	1.00	54.03
ATOM	730	CB	HIS	99	42.720	36.793	28.052	1.00	55.02
ATOM	731	CG	HIS	99	41.732	36.872	29.172	1.00	55.71
ATOM	732	CD2	HIS	99	40.682	37.704	29.373	1.00	55.66
ATOM	733	ND1	HIS	99	41.739	35.999	30.239	1.00	56.19
ATOM	734	CE1	HIS	99	40.736	36.288	31.049	1.00	56.30
ATOM	735	NE2	HIS	99	40.080	37.319	30.546	1.00	56.72
ATOM	736	C	HIS	99	44.445	38.082	29.351	1.00	53.46
ATOM	737	O	HIS	99	44.526	38.007	30.577	1.00	53.47

FIG. 4M

ATOM	738	N	GLN	100	44.583	39.214	28.683	1.00	52.94
ATOM	739	CA	GLN	100	44.841	40.468	29.349	1.00	53.34
ATOM	740	CB	GLN	100	46.354	40.649	29.513	1.00	53.39
ATOM	741	CG	GLN	100	46.790	42.001	30.055	1.00	54.26
ATOM	742	CD	GLN	100	46.168	42.345	31.394	1.00	54.43
ATOM	743	OE1	GLN	100	46.349	41.629	32.384	1.00	55.27
ATOM	744	NE2	GLN	100	45.433	43.452	31.432	1.00	53.60
ATOM	745	C	GLN	100	44.243	41.567	28.481	1.00	53.43
ATOM	746	O	GLN	100	44.416	41.569	27.260	1.00	53.75
ATOM	747	N	THR	101	43.527	42.493	29.105	1.00	52.90
ATOM	748	CA	THR	101	42.905	43.576	28.367	1.00	53.12
ATOM	749	CB	THR	101	41.495	43.826	28.894	1.00	52.52
ATOM	750	OG1	THR	101	40.789	42.582	28.925	1.00	52.85
ATOM	751	CG2	THR	101	40.752	44.808	27.999	1.00	52.23
ATOM	752	C	THR	101	43.731	44.845	28.499	1.00	53.61
ATOM	753	O	THR	101	44.285	45.108	29.563	1.00	53.95
ATOM	754	N	TYR	102	43.809	45.628	27.422	1.00	54.10
ATOM	755	CA	TYR	102	44.585	46.869	27.422	1.00	55.36
ATOM	756	CB	TYR	102	45.878	46.708	26.608	1.00	54.89
ATOM	757	CG	TYR	102	46.788	45.569	27.015	1.00	54.25
ATOM	758	CD1	TYR	102	46.382	44.241	26.888	1.00	54.08
ATOM	759	CE1	TYR	102	47.227	43.197	27.226	1.00	53.44
ATOM	760	CD2	TYR	102	48.069	45.822	27.497	1.00	53.79
ATOM	761	CE2	TYR	102	48.922	44.785	27.840	1.00	53.76
ATOM	762	CZ	TYR	102	48.498	43.475	27.701	1.00	53.85
ATOM	763	OH	TYR	102	49.355	42.442	28.021	1.00	54.03
ATOM	764	C	TYR	102	43.813	48.041	26.822	1.00	56.65
ATOM	765	O	TYR	102	43.173	47.899	25.781	1.00	56.91
ATOM	766	N	SER	103	43.891	49.203	27.462	1.00	58.50
ATOM	767	CA	SER	103	43.217	50.385	26.938	1.00	60.94
ATOM	768	CB	SER	103	42.997	51.411	28.049	1.00	61.09
ATOM	769	OG	SER	103	44.231	51.829	28.602	1.00	62.50
ATOM	770	C	SER	103	44.090	50.985	25.833	1.00	62.31
ATOM	771	O	SER	103	45.293	50.729	25.771	1.00	62.27
ATOM	772	N	ALA	104	43.487	51.783	24.960	1.00	64.47
ATOM	773	CA	ALA	104	44.226	52.386	23.856	1.00	67.01
ATOM	774	CB	ALA	104	43.516	52.093	22.526	1.00	67.01
ATOM	775	C	ALA	104	44.410	53.888	24.025	1.00	68.66
ATOM	776	O	ALA	104	43.458	54.658	23.902	1.00	69.01
ATOM	777	N	PRO	105	45.648	54.327	24.305	1.00	70.09
ATOM	778	CD	PRO	105	46.878	53.522	24.397	1.00	70.06
ATOM	779	CA	PRO	105	45.946	55.751	24.485	1.00	71.25
ATOM	780	CB	PRO	105	47.443	55.748	24.783	1.00	70.79
ATOM	781	CG	PRO	105	47.929	54.535	24.046	1.00	70.54
ATOM	782	C	PRO	105	45.592	56.586	23.251	1.00	72.81
ATOM	783	O	PRO	105	45.837	56.170	22.117	1.00	73.09
ATOM	784	N	GLU	106	45.012	57.762	23.479	1.00	74.39
ATOM	785	CA	GLU	106	44.619	58.652	22.391	1.00	76.25
ATOM	786	CB	GLU	106	43.991	59.921	22.950	1.00	76.77
ATOM	787	CG	GLU	106	42.702	59.673	23.680	1.00	78.35
ATOM	788	CD	GLU	106	42.397	60.775	24.657	1.00	79.28
ATOM	789	OE1	GLU	106	42.239	61.934	24.214	1.00	79.74
ATOM	790	OE2	GLU	106	42.326	60.478	25.871	1.00	80.03
ATOM	791	C	GLU	106	45.784	59.028	21.494	1.00	77.33
ATOM	792	O	GLU	106	45.600	59.262	20.300	1.00	77.48
ATOM	793	N	ASP	107	46.980	59.104	22.068	1.00	78.72
ATOM	794	CA	ASP	107	48.161	59.440	21.284	1.00	80.10

FIG. 4N

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ATOM    795  CB  ASP  107      49.431  59.316  22.134  1.00 80.44
ATOM    796  CG  ASP  107      49.965  57.889  22.185  1.00 81.03
ATOM    797  OD1 ASP  107      49.198  56.976  22.569  1.00 81.42
ATOM    798  OD2 ASP  107      51.151  57.682  21.839  1.00 80.86
ATOM    799  C   ASP  107      48.212  58.424  20.151  1.00 80.92
ATOM    800  O   ASP  107      48.724  58.703  19.065  1.00 81.29
ATOM    801  N   ALA  108      47.670  57.241  20.428  1.00 81.68
ATOM    802  CA  ALA  108      47.628  56.151  19.463  1.00 82.45
ATOM    803  CB  ALA  108      47.605  54.813  20.200  1.00 82.45
ATOM    804  C   ALA  108      46.406  56.275  18.553  1.00 82.91
ATOM    805  O   ALA  108      46.536  56.351  17.331  1.00 82.98
ATOM    806  N   MSE  109      45.221  56.303  19.157  1.00 83.41
ATOM    807  CA  MSE  109      43.974  56.414  18.407  1.00 83.78
ATOM    808  CB  MSE  109      42.787  56.519  19.368  1.00 85.45
ATOM    809  CG  MSE  109      41.581  55.678  18.972  1.00 87.01
ATOM    810  SE  MSE  109      41.933  53.898  19.096  1.00 90.12
ATOM    811  CE  MSE  109      42.665  53.581  17.453  1.00 88.95
ATOM    812  C   MSE  109      43.992  57.633  17.494  1.00 83.17
ATOM    813  O   MSE  109      43.235  57.710  16.527  1.00 83.19
ATOM    814  N   THR  110      44.854  58.590  17.820  1.00 82.51
ATOM    815  CA  THR  110      44.986  59.815  17.040  1.00 82.00
ATOM    816  CB  THR  110      45.289  61.022  17.949  1.00 82.44
ATOM    817  OG1 THR  110      44.302  61.103  18.986  1.00 83.00
ATOM    818  CG2 THR  110      45.283  62.313  17.142  1.00 82.69
ATOM    819  C   THR  110      46.150  59.640  16.082  1.00 81.25
ATOM    820  O   THR  110      46.127  60.123  14.949  1.00 80.95
ATOM    821  N   GLY  111      47.168  58.933  16.559  1.00 80.84
ATOM    822  CA  GLY  111      48.358  58.691  15.768  1.00 80.12
ATOM    823  C   GLY  111      48.121  57.986  14.450  1.00 79.53
ATOM    824  O   GLY  111      47.018  57.531  14.148  1.00 79.54
ATOM    825  N   THR  112      49.181  57.904  13.658  1.00 78.87
ATOM    826  CA  THR  112      49.129  57.254  12.360  1.00 78.09
ATOM    827  CB  THR  112      50.427  57.553  11.561  1.00 78.67
ATOM    828  OG1 THR  112      50.329  57.001  10.240  1.00 79.18
ATOM    829  CG2 THR  112      51.644  56.956  12.279  1.00 78.48
ATOM    830  C   THR  112      48.992  55.748  12.579  1.00 77.09
ATOM    831  O   THR  112      49.231  55.254  13.685  1.00 76.48
ATOM    832  N   ALA  113      48.601  55.027  11.529  1.00 76.26
ATOM    833  CA  ALA  113      48.443  53.573  11.603  1.00 75.60
ATOM    834  CB  ALA  113      48.184  53.001  10.208  1.00 76.00
ATOM    835  C   ALA  113      49.711  52.965  12.191  1.00 74.65
ATOM    836  O   ALA  113      49.665  52.006  12.968  1.00 74.58
ATOM    837  N   GLU  114      50.845  53.538  11.803  1.00 73.24
ATOM    838  CA  GLU  114      52.139  53.088  12.288  1.00 71.57
ATOM    839  CB  GLU  114      53.246  53.971  11.700  1.00 72.34
ATOM    840  CG  GLU  114      53.130  54.167  10.188  1.00 71.64
ATOM    841  CD  GLU  114      53.325  52.877   9.401  1.00 72.49
ATOM    842  OE1 GLU  114      53.192  51.781   9.994  1.00 72.24
ATOM    843  OE2 GLU  114      53.600  52.960   8.183  1.00 71.83
ATOM    844  C   GLU  114      52.085  53.233  13.801  1.00 70.37
ATOM    845  O   GLU  114      52.297  52.266  14.537  1.00 69.92
ATOM    846  N   MET  115      51.778  54.450  14.246  1.00 68.75
ATOM    847  CA  MET  115      51.657  54.760  15.669  1.00 66.97
ATOM    848  CB  MET  115      51.013  56.140  15.866  1.00 67.15
ATOM    849  CG  MET  115      51.999  57.277  16.040  1.00 66.94
ATOM    850  SD  MET  115      53.203  56.869  17.320  1.00 67.61
ATOM    851  CE  MET  115      52.137  56.732  18.788  1.00 66.65
```

FIG. 40

ATOM	852	C	MET	115	50.799	53.718	16.374	1.00	65.81
ATOM	853	O	MET	115	51.266	53.010	17.275	1.00	65.94
ATOM	854	N	LEU	116	49.542	53.635	15.940	1.00	63.70
ATOM	855	CA	LEU	116	48.561	52.711	16.504	1.00	61.63
ATOM	856	CB	LEU	116	47.287	52.720	15.650	1.00	60.89
ATOM	857	CG	LEU	116	45.948	52.226	16.205	1.00	59.42
ATOM	858	CD1	LEU	116	44.953	52.182	15.051	1.00	58.84
ATOM	859	CD2	LEU	116	46.081	50.858	16.847	1.00	58.86
ATOM	860	C	LEU	116	49.083	51.285	16.613	1.00	60.35
ATOM	861	O	LEU	116	48.977	50.665	17.667	1.00	60.48
ATOM	862	N	PHE	117	49.641	50.756	15.531	1.00	59.14
ATOM	863	CA	PHE	117	50.138	49.391	15.580	1.00	58.14
ATOM	864	CB	PHE	117	50.298	48.819	14.173	1.00	57.03
ATOM	865	CG	PHE	117	49.055	48.144	13.669	1.00	56.22
ATOM	866	CD1	PHE	117	48.005	48.889	13.143	1.00	55.49
ATOM	867	CD2	PHE	117	48.909	46.763	13.783	1.00	55.59
ATOM	868	CE1	PHE	117	46.830	48.270	12.741	1.00	55.25
ATOM	869	CE2	PHE	117	47.736	46.134	13.384	1.00	55.20
ATOM	870	CZ	PHE	117	46.695	46.887	12.862	1.00	55.23
ATOM	871	C	PHE	117	51.415	49.204	16.382	1.00	57.89
ATOM	872	O	PHE	117	51.799	48.073	16.690	1.00	57.80
ATOM	873	N	ALA	118	52.078	50.303	16.725	1.00	57.35
ATOM	874	CA	ALA	118	53.275	50.193	17.537	1.00	56.79
ATOM	875	CB	ALA	118	54.004	51.533	17.594	1.00	56.42
ATOM	876	C	ALA	118	52.747	49.792	18.922	1.00	56.46
ATOM	877	O	ALA	118	53.220	48.829	19.536	1.00	56.68
ATOM	878	N	ALA	119	51.733	50.515	19.391	1.00	55.57
ATOM	879	CA	ALA	119	51.142	50.226	20.693	1.00	55.05
ATOM	880	CB	ALA	119	49.931	51.135	20.952	1.00	53.91
ATOM	881	C	ALA	119	50.719	48.769	20.763	1.00	54.96
ATOM	882	O	ALA	119	51.090	48.052	21.698	1.00	54.94
ATOM	883	N	ILE	120	49.948	48.338	19.763	1.00	55.10
ATOM	884	CA	ILE	120	49.443	46.969	19.715	1.00	55.51
ATOM	885	CB	ILE	120	48.679	46.679	18.397	1.00	54.45
ATOM	886	CG2	ILE	120	47.922	45.363	18.525	1.00	53.30
ATOM	887	CG1	ILE	120	47.688	47.808	18.089	1.00	53.32
ATOM	888	CD1	ILE	120	46.871	47.581	16.820	1.00	51.70
ATOM	889	C	ILE	120	50.575	45.957	19.846	1.00	56.57
ATOM	890	O	ILE	120	50.477	45.006	20.632	1.00	56.52
ATOM	891	N	SER	121	51.645	46.169	19.076	1.00	57.78
ATOM	892	CA	SER	121	52.814	45.284	19.093	1.00	58.54
ATOM	893	CB	SER	121	53.844	45.730	18.045	1.00	58.96
ATOM	894	OG	SER	121	53.377	45.507	16.720	1.00	59.32
ATOM	895	C	SER	121	53.457	45.280	20.473	1.00	58.74
ATOM	896	O	SER	121	54.007	44.265	20.918	1.00	57.56
ATOM	897	N	GLU	122	53.379	46.422	21.151	1.00	59.50
ATOM	898	CA	GLU	122	53.947	46.529	22.484	1.00	60.44
ATOM	899	CB	GLU	122	54.003	47.986	22.941	1.00	60.60
ATOM	900	CG	GLU	122	55.104	48.241	23.952	1.00	60.45
ATOM	901	CD	GLU	122	54.706	49.252	25.003	1.00	61.76
ATOM	902	OE1	GLU	122	54.152	50.312	24.630	1.00	61.92
ATOM	903	OE2	GLU	122	54.950	48.986	26.202	1.00	62.20
ATOM	904	C	GLU	122	53.091	45.725	23.452	1.00	60.63
ATOM	905	O	GLU	122	53.565	44.761	24.048	1.00	60.82
ATOM	906	N	CYS	123	51.831	46.120	23.605	1.00	60.96
ATOM	907	CA	CYS	123	50.936	45.410	24.510	1.00	61.79
ATOM	908	CB	CYS	123	49.481	45.840	24.278	1.00	61.63

FIG. 4P

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ATOM    909  SG  CYS  123      49.191  47.636  24.439  1.00 62.83
ATOM    910  C   CYS  123      51.107  43.922  24.233  1.00 61.90
ATOM    911  O   CYS  123      51.028  43.095  25.147  1.00 61.89
ATOM    912  N   ILE  124      51.350  43.588  22.966  1.00 62.36
ATOM    913  CA  ILE  124      51.561  42.197  22.588  1.00 62.79
ATOM    914  CB  ILE  124      52.033  42.061  21.109  1.00 62.52
ATOM    915  CG2 ILE  124      52.618  40.676  20.877  1.00 61.07
ATOM    916  CG1 ILE  124      50.866  42.280  20.138  1.00 61.53
ATOM    917  CD1 ILE  124      50.016  41.038  19.888  1.00 61.77
ATOM    918  C   ILE  124      52.673  41.706  23.499  1.00 62.76
ATOM    919  O   ILE  124      52.475  40.807  24.320  1.00 62.23
ATOM    920  N   SER  125      53.839  42.327  23.347  1.00 63.43
ATOM    921  CA  SER  125      55.020  42.002  24.138  1.00 64.63
ATOM    922  CB  SER  125      56.062  43.117  23.986  1.00 65.05
ATOM    923  OG  SER  125      57.324  42.745  24.523  1.00 67.01
ATOM    924  C   SER  125      54.646  41.840  25.610  1.00 64.32
ATOM    925  O   SER  125      54.886  40.794  26.219  1.00 64.46
ATOM    926  N   ASP  126      54.047  42.884  26.169  1.00 64.43
ATOM    927  CA  ASP  126      53.626  42.894  27.562  1.00 64.86
ATOM    928  CB  ASP  126      52.660  44.060  27.788  1.00 64.95
ATOM    929  CG  ASP  126      52.390  44.323  29.253  1.00 65.38
ATOM    930  OD1 ASP  126      51.952  43.389  29.955  1.00 65.74
ATOM    931  OD2 ASP  126      52.613  45.467  29.706  1.00 65.92
ATOM    932  C   ASP  126      52.968  41.572  27.980  1.00 64.65
ATOM    933  O   ASP  126      53.424  40.918  28.924  1.00 64.28
ATOM    934  N   PHE  127      51.902  41.189  27.274  1.00 64.96
ATOM    935  CA  PHE  127      51.177  39.948  27.565  1.00 65.21
ATOM    936  CB  PHE  127      50.145  39.657  26.468  1.00 64.22
ATOM    937  CG  PHE  127      49.569  38.258  26.525  1.00 63.67
ATOM    938  CD1 PHE  127      48.774  37.857  27.594  1.00 63.64
ATOM    939  CD2 PHE  127      49.830  37.343  25.512  1.00 63.42
ATOM    940  CE1 PHE  127      48.247  36.564  27.652  1.00 63.40
ATOM    941  CE2 PHE  127      49.308  36.051  25.560  1.00 63.55
ATOM    942  CZ  PHE  127      48.516  35.661  26.632  1.00 63.49
ATOM    943  C   PHE  127      52.154  38.791  27.631  1.00 65.83
ATOM    944  O   PHE  127      52.195  38.030  28.600  1.00 65.71
ATOM    945  N   LEU  128      52.931  38.684  26.562  1.00 66.57
ATOM    946  CA  LEU  128      53.942  37.656  26.387  1.00 67.52
ATOM    947  CB  LEU  128      54.773  38.022  25.166  1.00 67.64
ATOM    948  CG  LEU  128      53.926  38.452  23.969  1.00 67.42
ATOM    949  CD1 LEU  128      54.819  39.108  22.941  1.00 67.90
ATOM    950  CD2 LEU  128      53.195  37.251  23.387  1.00 67.65
ATOM    951  C   LEU  128      54.850  37.502  27.609  1.00 68.09
ATOM    952  O   LEU  128      54.829  36.468  28.285  1.00 67.92
ATOM    953  N   ASP  129      55.654  38.530  27.878  1.00 68.62
ATOM    954  CA  ASP  129      56.565  38.514  29.018  1.00 69.22
ATOM    955  CB  ASP  129      57.135  39.907  29.287  1.00 68.93
ATOM    956  CG  ASP  129      58.115  40.342  28.239  1.00 68.90
ATOM    957  OD1 ASP  129      59.100  39.606  28.011  1.00 69.12
ATOM    958  OD2 ASP  129      57.900  41.423  27.650  1.00 69.22
ATOM    959  C   ASP  129      55.843  38.059  30.267  1.00 69.59
ATOM    960  O   ASP  129      56.063  36.956  30.761  1.00 69.41
ATOM    961  N   LYS  130      54.973  38.940  30.753  1.00 70.10
ATOM    962  CA  LYS  130      54.190  38.733  31.958  1.00 70.67
ATOM    963  CB  LYS  130      53.285  39.946  32.159  1.00 70.80
ATOM    964  CG  LYS  130      54.076  41.252  32.052  1.00 70.54
ATOM    965  CD  LYS  130      53.218  42.479  32.266  1.00 70.22
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FIG. 4Q

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ATOM    966  CE  LYS   130      54.021  43.746  32.011  1.00 70.07
ATOM    967  NZ  LYS   130      53.204  44.977  32.195  1.00 69.69
ATOM    968  C   LYS   130      53.394  37.441  31.982  1.00 71.17
ATOM    969  O   LYS   130      52.381  37.331  32.673  1.00 70.99
ATOM    970  N   HIS   131      53.883  36.468  31.221  1.00 72.01
ATOM    971  CA  HIS   131      53.301  35.139  31.125  1.00 73.44
ATOM    972  CB  HIS   131      52.313  35.065  29.965  1.00 73.00
ATOM    973  CG  HIS   131      50.881  35.076  30.397  1.00 72.93
ATOM    974  CD2 HIS   131      49.960  34.085  30.454  1.00 72.73
ATOM    975  ND1 HIS   131      50.256  36.210  30.869  1.00 72.87
ATOM    976  CE1 HIS   131      49.010  35.917  31.196  1.00 73.01
ATOM    977  NE2 HIS   131      48.806  34.634  30.954  1.00 73.04
ATOM    978  C   HIS   131      54.424  34.124  30.908  1.00 74.61
ATOM    979  O   HIS   131      54.419  33.049  31.514  1.00 74.70
ATOM    980  N   GLN   132      55.374  34.502  30.046  1.00 76.14
ATOM    981  CA  GLN   132      56.566  33.727  29.658  1.00 77.30
ATOM    982  CB  GLN   132      56.536  32.293  30.218  1.00 77.68
ATOM    983  CG  GLN   132      55.424  31.387  29.676  1.00 78.41
ATOM    984  CD  GLN   132      55.823  30.611  28.436  1.00 78.88
ATOM    985  OE1 GLN   132      56.016  31.179  27.356  1.00 78.50
ATOM    986  NE2 GLN   132      55.951  29.294  28.587  1.00 79.41
ATOM    987  C   GLN   132      56.673  33.682  28.134  1.00 77.86
ATOM    988  O   GLN   132      57.769  33.638  27.574  1.00 77.91
ATOM    989  N   MSE   133      55.520  33.703  27.472  1.00 78.39
ATOM    990  CA  MSE   133      55.450  33.662  26.017  1.00 78.88
ATOM    991  CB  MSE   133      53.989  33.684  25.551  1.00 80.96
ATOM    992  CG  MSE   133      53.278  32.347  25.586  1.00 83.34
ATOM    993  SE  MSE   133      51.991  32.273  26.846  1.00 87.09
ATOM    994  CE  MSE   133      52.168  30.521  27.421  1.00 84.33
ATOM    995  C   MSE   133      56.174  34.812  25.333  1.00 77.90
ATOM    996  O   MSE   133      55.552  35.548  24.567  1.00 78.34
ATOM    997  N   LYS   134      57.470  34.973  25.587  1.00 75.97
ATOM    998  CA  LYS   134      58.225  36.053  24.949  1.00 73.96
ATOM    999  CB  LYS   134      58.976  36.879  25.997  1.00 73.14
ATOM   1000  CG  LYS   134      59.676  38.125  25.454  1.00 72.28
ATOM   1001  CD  LYS   134      58.697  39.250  25.141  1.00 70.99
ATOM   1002  CE  LYS   134      59.415  40.586  24.935  1.00 70.06
ATOM   1003  NZ  LYS   134      60.234  40.640  23.687  1.00 69.46
ATOM   1004  C   LYS   134      59.211  35.443  23.964  1.00 72.94
ATOM   1005  O   LYS   134      59.727  36.123  23.077  1.00 72.63
ATOM   1006  N   HIS   135      59.457  34.148  24.132  1.00 72.28
ATOM   1007  CA  HIS   135      60.377  33.411  23.275  1.00 71.52
ATOM   1008  CB  HIS   135      61.359  32.584  24.119  1.00 71.15
ATOM   1009  CG  HIS   135      60.719  31.448  24.859  1.00 70.88
ATOM   1010  CD2 HIS   135      60.908  30.109  24.773  1.00 70.87
ATOM   1011  ND1 HIS   135      59.750  31.635  25.822  1.00 70.81
ATOM   1012  CE1 HIS   135      59.370  30.462  26.298  1.00 70.56
ATOM   1013  NE2 HIS   135      60.057  29.519  25.678  1.00 70.85
ATOM   1014  C   HIS   135      59.584  32.482  22.365  1.00 71.26
ATOM   1015  O   HIS   135      60.152  31.818  21.499  1.00 71.53
ATOM   1016  N   LYS   136      58.272  32.434  22.574  1.00 70.85
ATOM   1017  CA  LYS   136      57.393  31.590  21.766  1.00 70.33
ATOM   1018  CB  LYS   136      56.077  31.329  22.508  1.00 69.64
ATOM   1019  CG  LYS   136      56.225  30.694  23.886  1.00 68.45
ATOM   1020  CD  LYS   136      56.740  29.271  23.783  1.00 68.01
ATOM   1021  CE  LYS   136      56.698  28.560  25.128  1.00 67.56
ATOM   1022  NZ  LYS   136      55.303  28.356  25.623  1.00 66.87
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FIG. 4R

ATOM	1023	C	LYS	136	57.088	32.296	20.443	1.00	70.46
ATOM	1024	O	LYS	136	57.100	33.530	20.371	1.00	70.94
ATOM	1025	N	LYS	137	56.828	31.519	19.396	1.00	70.16
ATOM	1026	CA	LYS	137	56.505	32.096	18.096	1.00	69.80
ATOM	1027	CB	LYS	137	57.505	31.642	17.023	1.00	71.09
ATOM	1028	CG	LYS	137	57.602	30.132	16.801	1.00	71.73
ATOM	1029	CD	LYS	137	58.567	29.840	15.654	1.00	72.44
ATOM	1030	CE	LYS	137	58.915	28.363	15.545	1.00	72.39
ATOM	1031	NZ	LYS	137	59.919	28.136	14.463	1.00	72.59
ATOM	1032	C	LYS	137	55.097	31.685	17.702	1.00	68.73
ATOM	1033	O	LYS	137	54.799	31.476	16.524	1.00	69.92
ATOM	1034	N	LEU	138	54.243	31.579	18.716	1.00	66.57
ATOM	1035	CA	LEU	138	52.841	31.193	18.586	1.00	63.82
ATOM	1036	CB	LEU	138	52.057	31.788	19.748	1.00	63.11
ATOM	1037	CG	LEU	138	52.364	31.145	21.092	1.00	62.89
ATOM	1038	CD1	LEU	138	51.924	32.068	22.220	1.00	62.68
ATOM	1039	CD2	LEU	138	51.669	29.786	21.150	1.00	61.80
ATOM	1040	C	LEU	138	52.114	31.553	17.294	1.00	62.26
ATOM	1041	O	LEU	138	52.416	32.566	16.647	1.00	62.54
ATOM	1042	N	PRO	139	51.149	30.708	16.894	1.00	60.11
ATOM	1043	CD	PRO	139	50.841	29.394	17.489	1.00	59.82
ATOM	1044	CA	PRO	139	50.356	30.937	15.682	1.00	57.91
ATOM	1045	CB	PRO	139	49.761	29.564	15.398	1.00	58.05
ATOM	1046	CG	PRO	139	49.573	28.999	16.772	1.00	59.12
ATOM	1047	C	PRO	139	49.302	31.968	16.101	1.00	55.89
ATOM	1048	O	PRO	139	48.469	31.693	16.973	1.00	55.71
ATOM	1049	N	LEU	140	49.358	33.154	15.501	1.00	53.40
ATOM	1050	CA	LEU	140	48.440	34.237	15.850	1.00	50.78
ATOM	1051	CB	LEU	140	49.195	35.576	15.834	1.00	49.87
ATOM	1052	CG	LEU	140	48.452	36.893	16.091	1.00	49.01
ATOM	1053	CD1	LEU	140	49.414	37.933	16.646	1.00	48.17
ATOM	1054	CD2	LEU	140	47.825	37.389	14.801	1.00	48.88
ATOM	1055	C	LEU	140	47.169	34.359	15.018	1.00	49.13
ATOM	1056	O	LEU	140	47.211	34.368	13.785	1.00	49.12
ATOM	1057	N	GLY	141	46.040	34.441	15.722	1.00	46.93
ATOM	1058	CA	GLY	141	44.743	34.613	15.086	1.00	43.70
ATOM	1059	C	GLY	141	44.324	36.041	15.402	1.00	41.11
ATOM	1060	O	GLY	141	44.277	36.414	16.569	1.00	41.46
ATOM	1061	N	PHE	142	44.018	36.842	14.388	1.00	38.27
ATOM	1062	CA	PHE	142	43.659	38.232	14.629	1.00	36.42
ATOM	1063	CB	PHE	142	44.648	39.118	13.882	1.00	34.58
ATOM	1064	CG	PHE	142	44.403	40.593	14.037	1.00	33.28
ATOM	1065	CD1	PHE	142	43.941	41.124	15.229	1.00	32.86
ATOM	1066	CD2	PHE	142	44.702	41.465	12.992	1.00	32.75
ATOM	1067	CE1	PHE	142	43.784	42.505	15.375	1.00	32.95
ATOM	1068	CE2	PHE	142	44.551	42.845	13.125	1.00	31.57
ATOM	1069	CZ	PHE	142	44.094	43.365	14.313	1.00	32.24
ATOM	1070	C	PHE	142	42.224	38.652	14.300	1.00	36.83
ATOM	1071	O	PHE	142	41.843	38.801	13.124	1.00	36.76
ATOM	1072	N	THR	143	41.423	38.848	15.347	1.00	35.96
ATOM	1073	CA	THR	143	40.047	39.288	15.156	1.00	34.35
ATOM	1074	CB	THR	143	39.179	38.997	16.373	1.00	33.98
ATOM	1075	OG1	THR	143	38.947	37.586	16.472	1.00	33.45
ATOM	1076	CG2	THR	143	37.854	39.750	16.255	1.00	33.35
ATOM	1077	C	THR	143	40.081	40.793	14.964	1.00	33.92
ATOM	1078	O	THR	143	40.190	41.544	15.928	1.00	34.30
ATOM	1079	N	PHE	144	40.009	41.227	13.716	1.00	33.00

FIG. 4S

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ATOM   1080  CA  PHE  144      40.029  42.649  13.383  1.00 31.69
ATOM   1081  CB  PHE  144      40.891  42.842  12.132  1.00 29.18
ATOM   1082  CG  PHE  144      41.189  44.264  11.807  1.00 26.95
ATOM   1083  CD1 PHE  144      41.727  45.108  12.763  1.00 26.21
ATOM   1084  CD2 PHE  144      40.956  44.755  10.533  1.00 25.39
ATOM   1085  CE1 PHE  144      42.026  46.428  12.450  1.00 26.79
ATOM   1086  CE2 PHE  144      41.250  46.070  10.212  1.00 25.46
ATOM   1087  CZ  PHE  144      41.785  46.910  11.167  1.00 25.80
ATOM   1088  C   PHE  144      38.562  42.981  13.112  1.00 32.02
ATOM   1089  O   PHE  144      37.929  42.280  12.333  1.00 33.96
ATOM   1090  N   SER  145      38.025  44.027  13.744  1.00 32.29
ATOM   1091  CA  SER  145      36.602  44.387  13.600  1.00 31.56
ATOM   1092  CB  SER  145      35.993  44.689  14.968  1.00 31.79
ATOM   1093  OG  SER  145      35.997  43.539  15.790  1.00 33.15
ATOM   1094  C   SER  145      36.271  45.546  12.679  1.00 30.95
ATOM   1095  O   SER  145      35.601  46.508  13.082  1.00 30.63
ATOM   1096  N   PHE  146      36.723  45.456  11.439  1.00 30.27
ATOM   1097  CA  PHE  146      36.452  46.513  10.489  1.00 29.49
ATOM   1098  CB  PHE  146      37.573  47.541  10.535  1.00 29.01
ATOM   1099  CG  PHE  146      37.848  48.054  11.908  1.00 27.96
ATOM   1100  CD1 PHE  146      38.654  47.336  12.775  1.00 28.87
ATOM   1101  CD2 PHE  146      37.245  49.221  12.359  1.00 27.88
ATOM   1102  CE1 PHE  146      38.852  47.777  14.078  1.00 29.72
ATOM   1103  CE2 PHE  146      37.434  49.670  13.659  1.00 26.92
ATOM   1104  CZ  PHE  146      38.232  48.955  14.520  1.00 28.49
ATOM   1105  C   PHE  146      36.318  45.937   9.093  1.00 29.49
ATOM   1106  O   PHE  146      36.668  44.778   8.846  1.00 29.56
ATOM   1107  N   PRO  147      35.805  46.738   8.152  1.00 29.02
ATOM   1108  CD  PRO  147      35.452  48.167   8.211  1.00 28.09
ATOM   1109  CA  PRO  147      35.662  46.212   6.798  1.00 30.12
ATOM   1110  CB  PRO  147      34.852  47.309   6.099  1.00 28.65
ATOM   1111  CG  PRO  147      35.377  48.540   6.749  1.00 28.13
ATOM   1112  C   PRO  147      37.047  45.969   6.179  1.00 30.89
ATOM   1113  O   PRO  147      37.938  46.821   6.263  1.00 32.17
ATOM   1114  N   VAL  148      37.221  44.807   5.557  1.00 31.62
ATOM   1115  CA  VAL  148      38.499  44.453   4.957  1.00 32.00
ATOM   1116  CB  VAL  148      39.399  43.733   6.002  1.00 32.44
ATOM   1117  CG1 VAL  148      40.471  42.940   5.311  1.00 33.36
ATOM   1118  CG2 VAL  148      40.035  44.758   6.934  1.00 32.04
ATOM   1119  C   VAL  148      38.351  43.557   3.733  1.00 31.54
ATOM   1120  O   VAL  148      37.937  42.402   3.858  1.00 30.91
ATOM   1121  N   ALA  149      38.688  44.091   2.560  1.00 31.66
ATOM   1122  CA  ALA  149      38.610  43.316   1.324  1.00 32.33
ATOM   1123  CB  ALA  149      38.834  44.213   0.120  1.00 31.16
ATOM   1124  C   ALA  149      39.723  42.288   1.428  1.00 33.43
ATOM   1125  O   ALA  149      40.882  42.653   1.431  1.00 35.59
ATOM   1126  N   HIS  150      39.387  41.008   1.535  1.00 33.73
ATOM   1127  CA  HIS  150      40.410  39.980   1.666  1.00 33.88
ATOM   1128  CB  HIS  150      39.868  38.780   2.450  1.00 34.82
ATOM   1129  CG  HIS  150      39.879  38.961   3.933  1.00 35.58
ATOM   1130  CD2 HIS  150      40.344  38.162   4.921  1.00 36.49
ATOM   1131  ND1 HIS  150      39.329  40.061   4.555  1.00 36.45
ATOM   1132  CE1 HIS  150      39.454  39.930   5.865  1.00 36.79
ATOM   1133  NE2 HIS  150      40.067  38.786   6.114  1.00 36.38
ATOM   1134  C   HIS  150      40.960  39.442   0.353  1.00 34.39
ATOM   1135  O   HIS  150      40.245  39.364  -0.655  1.00 34.56
ATOM   1136  N   ALA  151      42.239  39.068   0.380  1.00 34.73
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FIG. 4T

ATOM	1137	CA	ALA	151	42.898	38.440	-0.762	1.00	34.53
ATOM	1138	CB	ALA	151	44.334	38.949	-0.919	1.00	34.86
ATOM	1139	C	ALA	151	42.894	36.968	-0.338	1.00	34.46
ATOM	1140	O	ALA	151	42.734	36.065	-1.161	1.00	34.16
ATOM	1141	N	ASP	152	43.050	36.754	0.970	1.00	34.36
ATOM	1142	CA	ASP	152	43.045	35.422	1.562	1.00	35.45
ATOM	1143	CB	ASP	152	44.335	34.687	1.214	1.00	37.69
ATOM	1144	CG	ASP	152	44.233	33.185	1.431	1.00	40.20
ATOM	1145	OD1	ASP	152	43.219	32.717	2.007	1.00	40.73
ATOM	1146	OD2	ASP	152	45.177	32.464	1.018	1.00	42.29
ATOM	1147	C	ASP	152	42.901	35.549	3.088	1.00	35.53
ATOM	1148	O	ASP	152	43.048	36.642	3.642	1.00	35.08
ATOM	1149	N	ILE	153	42.627	34.433	3.762	1.00	35.49
ATOM	1150	CA	ILE	153	42.436	34.427	5.213	1.00	35.75
ATOM	1151	CB	ILE	153	42.258	32.984	5.754	1.00	35.32
ATOM	1152	CG2	ILE	153	43.609	32.316	5.937	1.00	34.16
ATOM	1153	CG1	ILE	153	41.593	33.022	7.130	1.00	35.44
ATOM	1154	CD1	ILE	153	40.225	33.697	7.131	1.00	36.43
ATOM	1155	C	ILE	153	43.571	35.079	6.011	1.00	36.77
ATOM	1156	O	ILE	153	43.450	35.278	7.229	1.00	36.40
ATOM	1157	N	ASP	154	44.665	35.411	5.332	1.00	37.10
ATOM	1158	CA	ASP	154	45.815	36.003	6.000	1.00	37.27
ATOM	1159	CB	ASP	154	46.982	35.013	5.991	1.00	38.98
ATOM	1160	CG	ASP	154	47.795	35.079	4.703	1.00	41.58
ATOM	1161	OD1	ASP	154	47.215	34.890	3.605	1.00	42.46
ATOM	1162	OD2	ASP	154	49.022	35.331	4.789	1.00	42.65
ATOM	1163	C	ASP	154	46.233	37.287	5.307	1.00	36.74
ATOM	1164	O	ASP	154	47.360	37.751	5.471	1.00	37.07
ATOM	1165	N	ALA	155	45.328	37.865	4.531	1.00	35.91
ATOM	1166	CA	ALA	155	45.650	39.093	3.830	1.00	36.20
ATOM	1167	CB	ALA	155	46.522	38.771	2.621	1.00	36.22
ATOM	1168	C	ALA	155	44.412	39.864	3.387	1.00	36.20
ATOM	1169	O	ALA	155	43.490	39.289	2.820	1.00	36.87
ATOM	1170	N	GLY	156	44.402	41.168	3.642	1.00	36.26
ATOM	1171	CA	GLY	156	43.279	41.997	3.245	1.00	37.08
ATOM	1172	C	GLY	156	43.481	43.446	3.647	1.00	38.10
ATOM	1173	O	GLY	156	44.027	43.727	4.711	1.00	38.52
ATOM	1174	N	ILE	157	43.052	44.377	2.805	1.00	39.16
ATOM	1175	CA	ILE	157	43.203	45.789	3.125	1.00	41.42
ATOM	1176	CB	ILE	157	43.389	46.646	1.842	1.00	42.84
ATOM	1177	CG2	ILE	157	44.844	46.550	1.349	1.00	44.32
ATOM	1178	CG1	ILE	157	42.399	46.193	0.761	1.00	43.93
ATOM	1179	CD1	ILE	157	42.630	46.838	-0.615	1.00	44.55
ATOM	1180	C	ILE	157	42.010	46.331	3.921	1.00	42.26
ATOM	1181	O	ILE	157	40.864	45.912	3.732	1.00	42.28
ATOM	1182	N	LEU	158	42.300	47.259	4.824	1.00	42.54
ATOM	1183	CA	LEU	158	41.283	47.873	5.648	1.00	43.22
ATOM	1184	CB	LEU	158	41.928	48.504	6.884	1.00	44.12
ATOM	1185	CG	LEU	158	41.090	49.514	7.670	1.00	44.84
ATOM	1186	CD1	LEU	158	40.020	48.782	8.472	1.00	45.23
ATOM	1187	CD2	LEU	158	42.006	50.320	8.590	1.00	45.09
ATOM	1188	C	LEU	158	40.548	48.947	4.855	1.00	43.56
ATOM	1189	O	LEU	158	40.984	50.099	4.801	1.00	43.77
ATOM	1190	N	LEU	159	39.434	48.569	4.239	1.00	43.40
ATOM	1191	CA	LEU	159	38.634	49.508	3.465	1.00	43.01
ATOM	1192	CB	LEU	159	37.238	48.935	3.280	1.00	43.36
ATOM	1193	CG	LEU	159	37.279	47.599	2.539	1.00	43.44

FIG. 4U

```
ATOM   1194  CD1 LEU   159      36.020  46.808   2.829  1.00 44.00
ATOM   1195  CD2 LEU   159      37.443  47.857   1.050  1.00 42.93
ATOM   1196  C   LEU   159      38.564  50.879   4.139  1.00 42.62
ATOM   1197  O   LEU   159      38.745  51.905   3.488  1.00 43.03
ATOM   1198  N   ASN   160      38.297  50.902   5.440  1.00 42.20
ATOM   1199  CA  ASN   160      38.243  52.169   6.170  1.00 41.99
ATOM   1200  CB  ASN   160      37.347  53.197   5.447  1.00 42.23
ATOM   1201  CG  ASN   160      35.913  52.733   5.295  1.00 43.38
ATOM   1202  OD1 ASN   160      35.225  53.102   4.334  1.00 42.38
ATOM   1203  ND2 ASN   160      35.444  51.934   6.250  1.00 44.48
ATOM   1204  C   ASN   160      37.813  51.988   7.616  1.00 41.13
ATOM   1205  O   ASN   160      37.359  50.913   8.011  1.00 41.17
ATOM   1206  N   TRP   161      37.980  53.043   8.403  1.00 40.24
ATOM   1207  CA  TRP   161      37.652  53.004   9.824  1.00 39.69
ATOM   1208  CB  TRP   161      38.522  54.003  10.602  1.00 39.33
ATOM   1209  CG  TRP   161      39.987  53.640  10.769  1.00 39.07
ATOM   1210  CD2 TRP   161      40.527  52.469  11.411  1.00 38.63
ATOM   1211  CE2 TRP   161      41.931  52.616  11.438  1.00 38.27
ATOM   1212  CE3 TRP   161      39.960  51.317  11.972  1.00 38.43
ATOM   1213  CD1 TRP   161      41.060  54.417  10.436  1.00 38.40
ATOM   1214  NE1 TRP   161      42.228  53.812  10.840  1.00 38.42
ATOM   1215  CZ2 TRP   161      42.778  51.659  12.000  1.00 38.26
ATOM   1216  CZ3 TRP   161      40.809  50.357  12.538  1.00 38.07
ATOM   1217  CH2 TRP   161      42.200  50.540  12.545  1.00 38.37
ATOM   1218  C   TRP   161      36.196  53.301  10.150  1.00 39.07
ATOM   1219  O   TRP   161      35.578  54.193   9.562  1.00 39.38
ATOM   1220  N   THR   162      35.668  52.555  11.114  1.00 38.45
ATOM   1221  CA  THR   162      34.302  52.734  11.593  1.00 38.37
ATOM   1222  CB  THR   162      33.381  51.600  11.125  1.00 37.71
ATOM   1223  OG1 THR   162      33.926  50.338  11.548  1.00 37.02
ATOM   1224  CG2 THR   162      33.226  51.635   9.617  1.00 36.52
ATOM   1225  C   THR   162      34.357  52.702  13.121  1.00 38.24
ATOM   1226  O   THR   162      35.405  52.443  13.703  1.00 37.86
ATOM   1227  N   LYS   163      33.231  52.968  13.770  1.00 38.99
ATOM   1228  CA  LYS   163      33.192  52.941  15.222  1.00 39.72
ATOM   1229  CB  LYS   163      33.510  51.528  15.728  1.00 38.16
ATOM   1230  CG  LYS   163      32.467  50.487  15.311  1.00 36.62
ATOM   1231  CD  LYS   163      32.727  49.108  15.918  1.00 34.66
ATOM   1232  CE  LYS   163      33.829  48.349  15.195  1.00 33.22
ATOM   1233  NZ  LYS   163      34.068  47.031  15.850  1.00 32.19
ATOM   1234  C   LYS   163      34.142  53.956  15.848  1.00 40.71
ATOM   1235  O   LYS   163      34.690  53.723  16.931  1.00 40.69
ATOM   1236  N   GLY   164      34.338  55.076  15.156  1.00 41.81
ATOM   1237  CA  GLY   164      35.187  56.139  15.672  1.00 43.90
ATOM   1238  C   GLY   164      36.685  56.031  15.463  1.00 45.41
ATOM   1239  O   GLY   164      37.375  57.055  15.381  1.00 45.25
ATOM   1240  N   PHE   165      37.190  54.802  15.397  1.00 47.06
ATOM   1241  CA  PHE   165      38.613  54.560  15.197  1.00 48.70
ATOM   1242  CB  PHE   165      38.852  53.117  14.767  1.00 47.20
ATOM   1243  CG  PHE   165      39.290  52.222  15.870  1.00 45.64
ATOM   1244  CD1 PHE   165      38.443  51.937  16.929  1.00 45.87
ATOM   1245  CD2 PHE   165      40.544  51.632  15.833  1.00 45.19
ATOM   1246  CE1 PHE   165      38.840  51.064  17.945  1.00 46.28
ATOM   1247  CE2 PHE   165      40.952  50.763  16.834  1.00 45.80
ATOM   1248  CZ  PHE   165      40.098  50.475  17.896  1.00 45.96
ATOM   1249  C   PHE   165      39.250  55.471  14.154  1.00 50.94
ATOM   1250  O   PHE   165      38.633  55.823  13.143  1.00 50.36
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FIG. 4V

ATOM	1251	N	LYS	166	40.500	55.838	14.415	1.00	53.77
ATOM	1252	CA	LYS	166	41.275	56.680	13.514	1.00	56.56
ATOM	1253	CB	LYS	166	41.050	58.170	13.822	1.00	56.16
ATOM	1254	CG	LYS	166	39.720	58.697	13.290	1.00	56.44
ATOM	1255	CD	LYS	166	39.524	58.320	11.812	1.00	56.54
ATOM	1256	CE	LYS	166	38.131	58.694	11.305	1.00	56.74
ATOM	1257	NZ	LYS	166	37.863	58.198	9.922	1.00	56.86
ATOM	1258	C	LYS	166	42.751	56.322	13.640	1.00	58.33
ATOM	1259	O	LYS	166	43.180	55.747	14.651	1.00	58.69
ATOM	1260	N	ALA	167	43.510	56.647	12.597	1.00	59.76
ATOM	1261	CA	ALA	167	44.943	56.375	12.543	1.00	61.43
ATOM	1262	CB	ALA	167	45.220	54.901	12.834	1.00	60.92
ATOM	1263	C	ALA	167	45.401	56.725	11.137	1.00	62.76
ATOM	1264	O	ALA	167	45.147	55.967	10.197	1.00	63.38
ATOM	1265	N	SER	168	46.066	57.872	10.999	1.00	63.98
ATOM	1266	CA	SER	168	46.556	58.345	9.704	1.00	64.43
ATOM	1267	CB	SER	168	47.636	59.414	9.903	1.00	64.96
ATOM	1268	OG	SER	168	47.130	60.546	10.594	1.00	65.76
ATOM	1269	C	SER	168	47.115	57.216	8.846	1.00	64.59
ATOM	1270	O	SER	168	47.805	56.322	9.347	1.00	64.35
ATOM	1271	N	GLY	169	46.800	57.260	7.553	1.00	64.75
ATOM	1272	CA	GLY	169	47.280	56.245	6.632	1.00	65.55
ATOM	1273	C	GLY	169	47.158	54.821	7.142	1.00	65.88
ATOM	1274	O	GLY	169	48.151	54.097	7.255	1.00	65.72
ATOM	1275	N	ALA	170	45.936	54.416	7.465	1.00	66.32
ATOM	1276	CA	ALA	170	45.699	53.065	7.947	1.00	66.82
ATOM	1277	CB	ALA	170	44.930	53.100	9.256	1.00	66.65
ATOM	1278	C	ALA	170	44.890	52.346	6.879	1.00	67.02
ATOM	1279	O	ALA	170	45.209	51.226	6.477	1.00	67.31
ATOM	1280	N	GLU	171	43.847	53.017	6.410	1.00	66.85
ATOM	1281	CA	GLU	171	42.979	52.463	5.387	1.00	66.80
ATOM	1282	CB	GLU	171	41.705	53.292	5.287	1.00	67.90
ATOM	1283	CG	GLU	171	41.958	54.783	5.279	1.00	69.27
ATOM	1284	CD	GLU	171	40.850	55.552	4.590	1.00	70.17
ATOM	1285	OE1	GLU	171	40.789	55.506	3.340	1.00	70.45
ATOM	1286	OE2	GLU	171	40.038	56.191	5.296	1.00	70.67
ATOM	1287	C	GLU	171	43.666	52.427	4.032	1.00	65.92
ATOM	1288	O	GLU	171	44.469	53.301	3.711	1.00	66.22
ATOM	1289	N	GLY	172	43.339	51.408	3.242	1.00	64.69
ATOM	1290	CA	GLY	172	43.922	51.265	1.925	1.00	62.79
ATOM	1291	C	GLY	172	45.096	50.312	1.882	1.00	61.61
ATOM	1292	O	GLY	172	45.493	49.884	0.805	1.00	61.59
ATOM	1293	N	ASN	173	45.643	49.965	3.045	1.00	60.93
ATOM	1294	CA	ASN	173	46.800	49.065	3.115	1.00	60.42
ATOM	1295	CB	ASN	173	47.922	49.722	3.913	1.00	61.72
ATOM	1296	CG	ASN	173	48.035	51.201	3.631	1.00	62.78
ATOM	1297	OD1	ASN	173	48.367	51.605	2.515	1.00	63.29
ATOM	1298	ND2	ASN	173	47.741	52.024	4.637	1.00	63.06
ATOM	1299	C	ASN	173	46.463	47.747	3.771	1.00	59.26
ATOM	1300	O	ASN	173	45.440	47.624	4.430	1.00	59.57
ATOM	1301	N	ASN	174	47.336	46.763	3.598	1.00	58.79
ATOM	1302	CA	ASN	174	47.126	45.447	4.196	1.00	58.46
ATOM	1303	CB	ASN	174	48.264	44.495	3.793	1.00	57.45
ATOM	1304	CG	ASN	174	48.104	43.093	4.375	1.00	57.22
ATOM	1305	OD1	ASN	174	48.757	42.144	3.924	1.00	56.21
ATOM	1306	ND2	ASN	174	47.245	42.957	5.382	1.00	56.76
ATOM	1307	C	ASN	174	47.083	45.615	5.712	1.00	58.42

FIG. 4W

ATOM	1308	O	ASN	174	47.927	46.302	6.281	1.00	59.03
ATOM	1309	N	VAL	175	46.091	45.008	6.359	1.00	58.23
ATOM	1310	CA	VAL	175	45.966	45.106	7.809	1.00	57.79
ATOM	1311	CB	VAL	175	44.544	44.765	8.295	1.00	57.69
ATOM	1312	CG1	VAL	175	44.461	44.933	9.807	1.00	56.81
ATOM	1313	CG2	VAL	175	43.531	45.665	7.603	1.00	57.69
ATOM	1314	C	VAL	175	46.944	44.150	8.470	1.00	57.62
ATOM	1315	O	VAL	175	47.734	44.560	9.319	1.00	57.89
ATOM	1316	N	VAL	176	46.896	42.878	8.086	1.00	57.24
ATOM	1317	CA	VAL	176	47.818	41.904	8.660	1.00	57.25
ATOM	1318	CB	VAL	176	47.638	40.501	8.037	1.00	57.27
ATOM	1319	CG1	VAL	176	48.597	39.511	8.701	1.00	56.21
ATOM	1320	CG2	VAL	176	46.196	40.035	8.199	1.00	56.28
ATOM	1321	C	VAL	176	49.232	42.396	8.362	1.00	57.38
ATOM	1322	O	VAL	176	50.212	41.911	8.926	1.00	57.30
ATOM	1323	N	GLY	177	49.319	43.374	7.467	1.00	57.41
ATOM	1324	CA	GLY	177	50.605	43.939	7.103	1.00	57.60
ATOM	1325	C	GLY	177	51.135	44.878	8.170	1.00	57.50
ATOM	1326	O	GLY	177	52.171	44.605	8.781	1.00	58.09
ATOM	1327	N	LEU	178	50.425	45.982	8.396	1.00	56.68
ATOM	1328	CA	LEU	178	50.837	46.959	9.396	1.00	55.42
ATOM	1329	CB	LEU	178	49.710	47.968	9.646	1.00	55.02
ATOM	1330	CG	LEU	178	49.394	48.906	8.466	1.00	54.15
ATOM	1331	CD1	LEU	178	48.158	49.743	8.766	1.00	53.80
ATOM	1332	CD2	LEU	178	50.588	49.815	8.197	1.00	54.17
ATOM	1333	C	LEU	178	51.247	46.279	10.701	1.00	54.84
ATOM	1334	O	LEU	178	52.177	46.717	11.375	1.00	55.07
ATOM	1335	N	LEU	179	50.575	45.192	11.050	1.00	53.85
ATOM	1336	CA	LEU	179	50.917	44.491	12.274	1.00	53.57
ATOM	1337	CB	LEU	179	49.882	43.409	12.582	1.00	52.75
ATOM	1338	CG	LEU	179	50.099	42.671	13.907	1.00	52.23
ATOM	1339	CD1	LEU	179	49.689	43.580	15.056	1.00	51.63
ATOM	1340	CD2	LEU	179	49.286	41.381	13.935	1.00	51.34
ATOM	1341	C	LEU	179	52.286	43.845	12.128	1.00	54.26
ATOM	1342	O	LEU	179	53.070	43.796	13.075	1.00	54.60
ATOM	1343	N	ARG	180	52.576	43.343	10.932	1.00	54.59
ATOM	1344	CA	ARG	180	53.855	42.679	10.688	1.00	54.08
ATOM	1345	CB	ARG	180	53.824	41.911	9.357	1.00	52.59
ATOM	1346	CG	ARG	180	53.273	40.498	9.515	1.00	50.37
ATOM	1347	CD	ARG	180	53.276	39.702	8.223	1.00	47.24
ATOM	1348	NE	ARG	180	52.610	38.420	8.425	1.00	45.06
ATOM	1349	CZ	ARG	180	51.979	37.754	7.462	1.00	43.97
ATOM	1350	NH1	ARG	180	51.935	38.256	6.226	1.00	42.53
ATOM	1351	NH2	ARG	180	51.366	36.601	7.735	1.00	42.95
ATOM	1352	C	ARG	180	55.059	43.605	10.732	1.00	54.76
ATOM	1353	O	ARG	180	56.009	43.343	11.473	1.00	54.65
ATOM	1354	N	ASP	181	55.036	44.681	9.951	1.00	55.34
ATOM	1355	CA	ASP	181	56.169	45.593	9.972	1.00	56.60
ATOM	1356	CB	ASP	181	56.266	46.386	8.649	1.00	56.43
ATOM	1357	CG	ASP	181	55.132	47.382	8.448	1.00	55.64
ATOM	1358	OD1	ASP	181	54.658	47.483	7.294	1.00	55.20
ATOM	1359	OD2	ASP	181	54.734	48.076	9.416	1.00	55.23
ATOM	1360	C	ASP	181	56.115	46.514	11.199	1.00	57.64
ATOM	1361	O	ASP	181	56.510	47.685	11.153	1.00	57.96
ATOM	1362	N	ALA	182	55.634	45.947	12.303	1.00	57.87
ATOM	1363	CA	ALA	182	55.524	46.646	13.577	1.00	57.84
ATOM	1364	CB	ALA	182	54.078	47.048	13.836	1.00	58.19

FIG. 4X

ATOM	1365	C	ALA	182	56.013	45.683	14.657	1.00	57.83
ATOM	1366	O	ALA	182	56.681	46.094	15.611	1.00	58.32
ATOM	1367	N	ILE	183	55.669	44.404	14.505	1.00	57.35
ATOM	1368	CA	ILE	183	56.109	43.381	15.448	1.00	57.40
ATOM	1369	CB	ILE	183	55.374	42.036	15.233	1.00	56.09
ATOM	1370	CG2	ILE	183	56.025	40.932	16.074	1.00	55.25
ATOM	1371	CG1	ILE	183	53.904	42.174	15.628	1.00	55.30
ATOM	1372	CD1	ILE	183	53.115	40.881	15.505	1.00	54.14
ATOM	1373	C	ILE	183	57.600	43.164	15.199	1.00	58.51
ATOM	1374	O	ILE	183	58.294	42.531	16.002	1.00	59.24
ATOM	1375	N	LYS	184	58.093	43.689	14.077	1.00	59.04
ATOM	1376	CA	LYS	184	59.508	43.550	13.757	1.00	59.19
ATOM	1377	CB	LYS	184	59.719	43.243	12.268	1.00	59.15
ATOM	1378	CG	LYS	184	59.356	44.354	11.310	1.00	58.36
ATOM	1379	CD	LYS	184	59.566	43.897	9.868	1.00	58.59
ATOM	1380	CE	LYS	184	58.637	42.735	9.500	1.00	59.26
ATOM	1381	NZ	LYS	184	58.751	42.306	8.067	1.00	59.63
ATOM	1382	C	LYS	184	60.270	44.806	14.155	1.00	59.27
ATOM	1383	O	LYS	184	61.382	44.705	14.667	1.00	59.28
ATOM	1384	N	ARG	185	59.695	45.984	13.923	1.00	59.21
ATOM	1385	CA	ARG	185	60.383	47.211	14.331	1.00	59.69
ATOM	1386	CB	ARG	185	59.545	48.458	14.060	1.00	59.70
ATOM	1387	CG	ARG	185	59.278	48.772	12.610	1.00	60.85
ATOM	1388	CD	ARG	185	59.138	50.280	12.443	1.00	60.89
ATOM	1389	NE	ARG	185	58.121	50.628	11.459	1.00	62.26
ATOM	1390	CZ	ARG	185	56.819	50.403	11.620	1.00	61.84
ATOM	1391	NH1	ARG	185	56.372	49.828	12.731	1.00	61.22
ATOM	1392	NH2	ARG	185	55.966	50.754	10.666	1.00	62.23
ATOM	1393	C	ARG	185	60.574	47.104	15.836	1.00	60.41
ATOM	1394	O	ARG	185	61.630	47.430	16.384	1.00	60.45
ATOM	1395	N	ARG	186	59.518	46.633	16.489	1.00	61.07
ATOM	1396	CA	ARG	186	59.489	46.460	17.933	1.00	61.42
ATOM	1397	CB	ARG	186	58.066	46.055	18.358	1.00	61.16
ATOM	1398	CG	ARG	186	57.666	46.433	19.786	1.00	61.08
ATOM	1399	CD	ARG	186	58.249	45.473	20.828	1.00	60.87
ATOM	1400	NE	ARG	186	57.917	45.894	22.188	1.00	61.44
ATOM	1401	CZ	ARG	186	58.294	45.246	23.288	1.00	60.67
ATOM	1402	NH1	ARG	186	59.024	44.133	23.201	1.00	60.28
ATOM	1403	NH2	ARG	186	57.942	45.712	24.481	1.00	61.46
ATOM	1404	C	ARG	186	60.516	45.399	18.344	1.00	61.85
ATOM	1405	O	ARG	186	60.980	44.610	17.514	1.00	62.16
ATOM	1406	N	GLY	187	60.873	45.401	19.628	1.00	62.07
ATOM	1407	CA	GLY	187	61.843	44.455	20.157	1.00	62.22
ATOM	1408	C	GLY	187	61.591	43.017	19.754	1.00	62.50
ATOM	1409	O	GLY	187	60.541	42.692	19.202	1.00	62.37
ATOM	1410	N	ASP	188	62.556	42.148	20.036	1.00	63.08
ATOM	1411	CA	ASP	188	62.414	40.746	19.684	1.00	62.67
ATOM	1412	CB	ASP	188	63.465	39.873	20.373	1.00	61.80
ATOM	1413	CG	ASP	188	63.027	38.409	20.468	1.00	60.64
ATOM	1414	OD1	ASP	188	62.125	38.107	21.289	1.00	60.77
ATOM	1415	OD2	ASP	188	63.565	37.563	19.715	1.00	60.43
ATOM	1416	C	ASP	188	61.047	40.193	20.022	1.00	63.58
ATOM	1417	O	ASP	188	60.441	40.539	21.044	1.00	62.69
ATOM	1418	N	PHE	189	60.599	39.309	19.138	1.00	64.49
ATOM	1419	CA	PHE	189	59.327	38.632	19.249	1.00	64.75
ATOM	1420	CB	PHE	189	58.233	39.629	19.598	1.00	64.84
ATOM	1421	CG	PHE	189	56.886	39.010	19.689	1.00	65.46

FIG. 4Y

```
ATOM   1422  CD1 PHE   189      56.707  37.824  20.402  1.00 65.54
ATOM   1423  CD2 PHE   189      55.795  39.592  19.052  1.00 65.28
ATOM   1424  CE1 PHE   189      55.455  37.224  20.481  1.00 65.61
ATOM   1425  CE2 PHE   189      54.542  39.007  19.122  1.00 65.71
ATOM   1426  CZ  PHE   189      54.369  37.819  19.839  1.00 65.57
ATOM   1427  C   PHE   189      59.018  37.952  17.919  1.00 65.33
ATOM   1428  O   PHE   189      58.921  38.609  16.881  1.00 64.91
ATOM   1429  N   GLU   190      58.879  36.631  17.956  1.00 66.13
ATOM   1430  CA  GLU   190      58.584  35.854  16.752  1.00 66.57
ATOM   1431  CB  GLU   190      59.387  34.545  16.755  1.00 66.34
ATOM   1432  CG  GLU   190      60.778  34.649  17.389  1.00 64.66
ATOM   1433  CD  GLU   190      61.908  34.356  16.411  1.00 64.02
ATOM   1434  OE1 GLU   190      63.054  34.161  16.874  1.00 63.09
ATOM   1435  OE2 GLU   190      61.658  34.327  15.186  1.00 63.04
ATOM   1436  C   GLU   190      57.093  35.528  16.745  1.00 67.09
ATOM   1437  O   GLU   190      56.609  34.828  17.638  1.00 67.36
ATOM   1438  N   MSE   191      56.367  36.030  15.747  1.00 67.05
ATOM   1439  CA  MSE   191      54.928  35.775  15.666  1.00 66.65
ATOM   1440  CB  MSE   191      54.164  36.920  16.347  1.00 69.47
ATOM   1441  CG  MSE   191      52.867  36.492  17.037  1.00 72.30
ATOM   1442  SE  MSE   191      53.120  35.293  18.409  1.00 78.56
ATOM   1443  CE  MSE   191      51.941  35.893  19.581  1.00 75.88
ATOM   1444  C   MSE   191      54.412  35.590  14.230  1.00 64.85
ATOM   1445  O   MSE   191      54.399  36.538  13.435  1.00 64.30
ATOM   1446  N   ASP   192      53.977  34.368  13.910  1.00 62.82
ATOM   1447  CA  ASP   192      53.449  34.051  12.580  1.00 60.76
ATOM   1448  CB  ASP   192      53.774  32.607  12.207  1.00 61.24
ATOM   1449  CG  ASP   192      55.210  32.427  11.792  1.00 61.76
ATOM   1450  OD1 ASP   192      55.684  33.219  10.947  1.00 62.45
ATOM   1451  OD2 ASP   192      55.863  31.492  12.299  1.00 62.32
ATOM   1452  C   ASP   192      51.942  34.266  12.459  1.00 59.03
ATOM   1453  O   ASP   192      51.143  33.375  12.767  1.00 58.37
ATOM   1454  N   VAL   193      51.567  35.453  11.991  1.00 57.00
ATOM   1455  CA  VAL   193      50.167  35.818  11.818  1.00 54.85
ATOM   1456  CB  VAL   193      50.034  37.305  11.454  1.00 55.09
ATOM   1457  CG1 VAL   193      48.568  37.712  11.448  1.00 54.84
ATOM   1458  CG2 VAL   193      50.826  38.146  12.441  1.00 54.87
ATOM   1459  C   VAL   193      49.473  34.977  10.746  1.00 53.19
ATOM   1460  O   VAL   193      49.500  35.303   9.555  1.00 52.03
ATOM   1461  N   VAL   194      48.854  33.894  11.205  1.00 51.82
ATOM   1462  CA  VAL   194      48.126  32.949  10.367  1.00 50.66
ATOM   1463  CB  VAL   194      47.841  31.644  11.174  1.00 51.08
ATOM   1464  CG1 VAL   194      46.686  30.860  10.554  1.00 52.09
ATOM   1465  CG2 VAL   194      49.091  30.778  11.211  1.00 51.33
ATOM   1466  C   VAL   194      46.798  33.498   9.808  1.00 49.99
ATOM   1467  O   VAL   194      46.677  33.726   8.602  1.00 49.40
ATOM   1468  N   ALA   195      45.813  33.723  10.683  1.00 48.93
ATOM   1469  CA  ALA   195      44.499  34.193  10.251  1.00 47.60
ATOM   1470  CB  ALA   195      43.467  33.123  10.572  1.00 47.58
ATOM   1471  C   ALA   195      43.992  35.546  10.760  1.00 46.68
ATOM   1472  O   ALA   195      44.344  35.996  11.851  1.00 46.16
ATOM   1473  N   MSE   196      43.157  36.182   9.940  1.00 45.43
ATOM   1474  CA  MSE   196      42.521  37.459  10.279  1.00 44.60
ATOM   1475  CB  MSE   196      43.079  38.623   9.451  1.00 45.32
ATOM   1476  CG  MSE   196      42.329  39.925   9.716  1.00 47.29
ATOM   1477  SE  MSE   196      42.937  41.426   8.852  1.00 53.21
ATOM   1478  CE  MSE   196      44.264  41.920   9.982  1.00 51.44
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FIG. 4Z

```
ATOM   1479  C   MSE  196      41.019  37.333  10.002  1.00 43.09
ATOM   1480  O   MSE  196      40.610  36.973   8.892  1.00 43.71
ATOM   1481  N   VAL  197      40.190  37.631  10.996  1.00 40.47
ATOM   1482  CA  VAL  197      38.751  37.514  10.799  1.00 37.00
ATOM   1483  CB  VAL  197      38.240  36.228  11.458  1.00 37.31
ATOM   1484  CG1 VAL  197      38.840  35.004  10.766  1.00 36.64
ATOM   1485  CG2 VAL  197      38.643  36.217  12.914  1.00 36.88
ATOM   1486  C   VAL  197      37.991  38.710  11.354  1.00 35.22
ATOM   1487  O   VAL  197      38.561  39.544  12.057  1.00 35.21
ATOM   1488  N   ASN  198      36.708  38.801  11.015  1.00 33.39
ATOM   1489  CA  ASN  198      35.830  39.883  11.491  1.00 30.23
ATOM   1490  CB  ASN  198      34.740  40.175  10.446  1.00 30.65
ATOM   1491  CG  ASN  198      33.801  41.309  10.852  1.00 31.35
ATOM   1492  OD1 ASN  198      32.907  41.128  11.686  1.00 32.70
ATOM   1493  ND2 ASN  198      33.997  42.486  10.251  1.00 30.53
ATOM   1494  C   ASN  198      35.217  39.356  12.780  1.00 28.41
ATOM   1495  O   ASN  198      35.052  38.143  12.937  1.00 26.14
ATOM   1496  N   ASP  199      34.892  40.252  13.711  1.00 27.77
ATOM   1497  CA  ASP  199      34.325  39.816  14.990  1.00 26.87
ATOM   1498  CB  ASP  199      34.156  41.007  15.945  1.00 26.75
ATOM   1499  CG  ASP  199      33.254  42.097  15.396  1.00 26.24
ATOM   1500  OD1 ASP  199      33.221  42.292  14.167  1.00 26.90
ATOM   1501  OD2 ASP  199      32.587  42.777  16.205  1.00 26.19
ATOM   1502  C   ASP  199      33.027  39.034  14.843  1.00 26.43
ATOM   1503  O   ASP  199      32.715  38.188  15.684  1.00 27.02
ATOM   1504  N   THR  200      32.291  39.292  13.763  1.00 25.45
ATOM   1505  CA  THR  200      31.050  38.585  13.510  1.00 25.65
ATOM   1506  CB  THR  200      30.261  39.193  12.339  1.00 25.75
ATOM   1507  OG1 THR  200      31.008  39.044  11.130  1.00 26.04
ATOM   1508  CG2 THR  200      30.002  40.672  12.573  1.00 26.48
ATOM   1509  C   THR  200      31.383  37.155  13.143  1.00 26.96
ATOM   1510  O   THR  200      30.832  36.211  13.712  1.00 27.62
ATOM   1511  N   VAL  201      32.295  36.990  12.189  1.00 28.07
ATOM   1512  CA  VAL  201      32.695  35.654  11.742  1.00 28.50
ATOM   1513  CB  VAL  201      33.785  35.726  10.665  1.00 29.26
ATOM   1514  CG1 VAL  201      34.056  34.332  10.123  1.00 31.22
ATOM   1515  CG2 VAL  201      33.370  36.684   9.546  1.00 27.90
ATOM   1516  C   VAL  201      33.231  34.818  12.901  1.00 29.16
ATOM   1517  O   VAL  201      32.816  33.676  13.101  1.00 29.44
ATOM   1518  N   ALA  202      34.156  35.395  13.663  1.00 30.31
ATOM   1519  CA  ALA  202      34.752  34.710  14.812  1.00 32.23
ATOM   1520  CB  ALA  202      35.591  35.705  15.643  1.00 31.72
ATOM   1521  C   ALA  202      33.688  34.070  15.696  1.00 33.37
ATOM   1522  O   ALA  202      33.789  32.894  16.073  1.00 34.14
ATOM   1523  N   THR  203      32.667  34.858  16.019  1.00 34.41
ATOM   1524  CA  THR  203      31.566  34.422  16.870  1.00 35.37
ATOM   1525  CB  THR  203      30.614  35.604  17.117  1.00 36.27
ATOM   1526  OG1 THR  203      31.370  36.708  17.645  1.00 37.04
ATOM   1527  CG2 THR  203      29.500  35.213  18.090  1.00 35.19
ATOM   1528  C   THR  203      30.800  33.260  16.242  1.00 36.08
ATOM   1529  O   THR  203      30.538  32.241  16.891  1.00 35.34
ATOM   1530  N   MSE  204      30.433  33.415  14.978  1.00 36.89
ATOM   1531  CA  MSE  204      29.722  32.348  14.299  1.00 37.94
ATOM   1532  CB  MSE  204      29.582  32.665  12.811  1.00 39.76
ATOM   1533  CG  MSE  204      29.065  31.504  11.954  1.00 40.74
ATOM   1534  SE  MSE  204      29.135  31.967  10.181  1.00 45.75
ATOM   1535  CE  MSE  204      30.643  31.057   9.627  1.00 45.26
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FIG. 4AA

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ATOM   1536  C   MSE  204      30.531  31.075  14.465  1.00 38.36
ATOM   1537  O   MSE  204      30.024  30.064  14.954  1.00 37.86
ATOM   1538  N   ILE  205      31.798  31.148  14.061  1.00 38.79
ATOM   1539  CA  ILE  205      32.696  30.008  14.137  1.00 40.09
ATOM   1540  CB  ILE  205      34.178  30.451  13.981  1.00 39.81
ATOM   1541  CG2 ILE  205      35.098  29.240  14.072  1.00 39.47
ATOM   1542  CG1 ILE  205      34.398  31.112  12.616  1.00 39.46
ATOM   1543  CD1 ILE  205      34.250  30.158  11.425  1.00 39.34
ATOM   1544  C   ILE  205      32.527  29.215  15.440  1.00 41.34
ATOM   1545  O   ILE  205      32.121  28.050  15.408  1.00 41.41
ATOM   1546  N   SER  206      32.812  29.830  16.584  1.00 42.01
ATOM   1547  CA  SER  206      32.683  29.112  17.849  1.00 43.71
ATOM   1548  CB  SER  206      32.999  30.038  19.013  1.00 43.57
ATOM   1549  OG  SER  206      32.149  31.163  18.971  1.00 44.54
ATOM   1550  C   SER  206      31.306  28.494  18.056  1.00 44.83
ATOM   1551  O   SER  206      31.185  27.304  18.364  1.00 45.40
ATOM   1552  N   CYS  207      30.260  29.291  17.894  1.00 46.32
ATOM   1553  CA  CYS  207      28.912  28.764  18.079  1.00 48.14
ATOM   1554  CB  CYS  207      27.869  29.842  17.780  1.00 46.74
ATOM   1555  SG  CYS  207      27.946  31.264  18.883  1.00 42.50
ATOM   1556  C   CYS  207      28.666  27.551  17.186  1.00 50.79
ATOM   1557  O   CYS  207      27.715  26.799  17.403  1.00 50.97
ATOM   1558  N   TYR  208      29.533  27.361  16.190  1.00 53.91
ATOM   1559  CA  TYR  208      29.418  26.243  15.247  1.00 56.61
ATOM   1560  CB  TYR  208      30.350  26.458  14.045  1.00 56.96
ATOM   1561  CG  TYR  208      30.370  25.303  13.062  1.00 57.29
ATOM   1562  CD1 TYR  208      29.307  25.090  12.182  1.00 57.54
ATOM   1563  CE1 TYR  208      29.319  24.026  11.280  1.00 57.47
ATOM   1564  CD2 TYR  208      31.448  24.418  13.019  1.00 57.54
ATOM   1565  CE2 TYR  208      31.468  23.350  12.125  1.00 57.60
ATOM   1566  CZ  TYR  208      30.404  23.163  11.258  1.00 57.47
ATOM   1567  OH  TYR  208      30.435  22.126  10.360  1.00 57.71
ATOM   1568  C   TYR  208      29.705  24.867  15.854  1.00 58.12
ATOM   1569  O   TYR  208      28.874  23.960  15.773  1.00 58.61
ATOM   1570  N   TYR  209      30.876  24.699  16.459  1.00 59.77
ATOM   1571  CA  TYR  209      31.198  23.399  17.028  1.00 61.36
ATOM   1572  CB  TYR  209      32.619  23.394  17.581  1.00 63.23
ATOM   1573  CG  TYR  209      33.648  23.401  16.472  1.00 65.26
ATOM   1574  CD1 TYR  209      34.058  24.595  15.876  1.00 66.13
ATOM   1575  CE1 TYR  209      34.959  24.594  14.807  1.00 67.31
ATOM   1576  CD2 TYR  209      34.165  22.206  15.973  1.00 65.88
ATOM   1577  CE2 TYR  209      35.062  22.193  14.906  1.00 66.79
ATOM   1578  CZ  TYR  209      35.457  23.386  14.328  1.00 67.37
ATOM   1579  OH  TYR  209      36.350  23.370  13.277  1.00 67.62
ATOM   1580  C   TYR  209      30.206  22.965  18.083  1.00 61.32
ATOM   1581  O   TYR  209      30.048  21.771  18.336  1.00 61.19
ATOM   1582  N   GLU  210      29.523  23.938  18.680  1.00 61.63
ATOM   1583  CA  GLU  210      28.524  23.658  19.701  1.00 61.05
ATOM   1584  CB  GLU  210      28.444  24.808  20.706  1.00 62.29
ATOM   1585  CG  GLU  210      27.539  24.499  21.884  1.00 65.45
ATOM   1586  CD  GLU  210      27.716  25.463  23.050  1.00 67.38
ATOM   1587  OE1 GLU  210      28.865  25.609  23.535  1.00 68.93
ATOM   1588  OE2 GLU  210      26.707  26.065  23.488  1.00 67.92
ATOM   1589  C   GLU  210      27.175  23.459  19.026  1.00 60.04
ATOM   1590  O   GLU  210      26.255  22.901  19.618  1.00 59.93
ATOM   1591  N   ASP  211      27.073  23.920  17.780  1.00 58.82
ATOM   1592  CA  ASP  211      25.849  23.797  16.984  1.00 57.80
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FIG. 4BB

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ATOM   1593  CB  ASP  211      24.804  24.824  17.441  1.00 58.16
ATOM   1594  CG  ASP  211      23.504  24.730  16.653  1.00 58.25
ATOM   1595  OD1 ASP  211      22.490  25.299  17.111  1.00 57.88
ATOM   1596  OD2 ASP  211      23.495  24.096  15.572  1.00 58.65
ATOM   1597  C   ASP  211      26.173  23.993  15.503  1.00 56.54
ATOM   1598  O   ASP  211      26.351  25.116  15.037  1.00 56.17
ATOM   1599  N   HIS  212      26.234  22.884  14.773  1.00 55.81
ATOM   1600  CA  HIS  212      26.577  22.884  13.351  1.00 55.26
ATOM   1601  CB  HIS  212      26.699  21.442  12.852  1.00 57.87
ATOM   1602  CG  HIS  212      27.816  20.678  13.493  1.00 61.52
ATOM   1603  CD2 HIS  212      27.815  19.527  14.205  1.00 62.63
ATOM   1604  ND1 HIS  212      29.127  21.110  13.460  1.00 62.80
ATOM   1605  CE1 HIS  212      29.884  20.258  14.127  1.00 63.70
ATOM   1606  NE2 HIS  212      29.114  19.288  14.590  1.00 63.71
ATOM   1607  C   HIS  212      25.665  23.656  12.412  1.00 53.29
ATOM   1608  O   HIS  212      26.014  23.883  11.251  1.00 52.77
ATOM   1609  N   GLN  213      24.496  24.058  12.895  1.00 51.08
ATOM   1610  CA  GLN  213      23.579  24.790  12.037  1.00 48.22
ATOM   1611  CB  GLN  213      22.135  24.347  12.298  1.00 49.39
ATOM   1612  CG  GLN  213      21.957  22.839  12.130  1.00 50.76
ATOM   1613  CD  GLN  213      20.507  22.410  11.965  1.00 51.82
ATOM   1614  OE1 GLN  213      19.653  22.721  12.803  1.00 52.48
ATOM   1615  NE2 GLN  213      20.223  21.679  10.883  1.00 51.72
ATOM   1616  C   GLN  213      23.746  26.289  12.202  1.00 45.19
ATOM   1617  O   GLN  213      22.978  27.077  11.654  1.00 45.00
ATOM   1618  N   CYS  214      24.759  26.686  12.957  1.00 41.87
ATOM   1619  CA  CYS  214      25.015  28.105  13.122  1.00 39.08
ATOM   1620  CB  CYS  214      25.907  28.386  14.332  1.00 39.18
ATOM   1621  SG  CYS  214      26.281  30.175  14.542  1.00 40.32
ATOM   1622  C   CYS  214      25.743  28.530  11.859  1.00 36.43
ATOM   1623  O   CYS  214      26.915  28.214  11.689  1.00 36.06
ATOM   1624  N   GLU  215      25.046  29.223  10.967  1.00 33.00
ATOM   1625  CA  GLU  215      25.664  29.672   9.736  1.00 30.60
ATOM   1626  CB  GLU  215      25.056  28.960   8.541  1.00 31.95
ATOM   1627  CG  GLU  215      25.289  27.466   8.561  1.00 33.57
ATOM   1628  CD  GLU  215      24.973  26.827   7.233  1.00 35.80
ATOM   1629  OE1 GLU  215      25.719  27.094   6.264  1.00 37.32
ATOM   1630  OE2 GLU  215      23.978  26.064   7.156  1.00 37.21
ATOM   1631  C   GLU  215      25.518  31.162   9.563  1.00 28.84
ATOM   1632  O   GLU  215      25.665  31.687   8.459  1.00 28.39
ATOM   1633  N   VAL  216      25.243  31.847  10.669  1.00 26.45
ATOM   1634  CA  VAL  216      25.083  33.291  10.648  1.00 23.67
ATOM   1635  CB  VAL  216      23.589  33.706  10.607  1.00 23.44
ATOM   1636  CG1 VAL  216      23.485  35.214  10.492  1.00 22.72
ATOM   1637  CG2 VAL  216      22.875  33.031   9.449  1.00 22.30
ATOM   1638  C   VAL  216      25.671  33.858  11.921  1.00 22.20
ATOM   1639  O   VAL  216      25.444  33.328  13.006  1.00 22.86
ATOM   1640  N   GLY  217      26.423  34.939  11.793  1.00 21.40
ATOM   1641  CA  GLY  217      26.997  35.554  12.965  1.00 21.14
ATOM   1642  C   GLY  217      26.524  36.994  13.022  1.00 22.30
ATOM   1643  O   GLY  217      26.432  37.677  11.983  1.00 22.05
ATOM   1644  N   MSE  218      26.201  37.454  14.228  1.00 23.03
ATOM   1645  CA  MSE  218      25.748  38.815  14.414  1.00 23.03
ATOM   1646  CB  MSE  218      24.208  38.880  14.445  1.00 25.98
ATOM   1647  CG  MSE  218      23.647  40.306  14.646  1.00 28.99
ATOM   1648  SE  MSE  218      21.806  40.486  14.543  1.00 35.34
ATOM   1649  CE  MSE  218      21.273  39.804  16.207  1.00 31.95
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FIG. 4CC

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ATOM   1650  C   MSE  218      26.320  39.405  15.694  1.00 21.99
ATOM   1651  O   MSE  218      26.425  38.738  16.724  1.00 22.34
ATOM   1652  N   ILE  219      26.694  40.670  15.606  1.00 21.28
ATOM   1653  CA  ILE  219      27.240  41.402  16.720  1.00 20.85
ATOM   1654  CB  ILE  219      28.702  41.840  16.449  1.00 20.74
ATOM   1655  CG2 ILE  219      29.164  42.757  17.558  1.00 19.65
ATOM   1656  CG1 ILE  219      29.623  40.627  16.335  1.00 19.32
ATOM   1657  CD1 ILE  219      29.656  39.770  17.596  1.00 20.63
ATOM   1658  C   ILE  219      26.413  42.676  16.838  1.00 21.47
ATOM   1659  O   ILE  219      26.297  43.431  15.868  1.00 21.30
ATOM   1660  N   VAL  220      25.823  42.908  18.003  1.00 21.91
ATOM   1661  CA  VAL  220      25.059  44.135  18.224  1.00 22.49
ATOM   1662  CB  VAL  220      23.563  43.873  18.479  1.00 22.04
ATOM   1663  CG1 VAL  220      22.815  45.183  18.425  1.00 21.50
ATOM   1664  CG2 VAL  220      23.007  42.901  17.463  1.00 22.03
ATOM   1665  C   VAL  220      25.650  44.775  19.477  1.00 23.27
ATOM   1666  O   VAL  220      25.095  44.642  20.575  1.00 23.94
ATOM   1667  N   GLY  221      26.795  45.436  19.312  1.00 22.78
ATOM   1668  CA  GLY  221      27.448  46.063  20.443  1.00 22.86
ATOM   1669  C   GLY  221      27.728  47.509  20.138  1.00 23.75
ATOM   1670  O   GLY  221      26.816  48.264  19.828  1.00 25.09
ATOM   1671  N   THR  222      28.988  47.906  20.233  1.00 24.06
ATOM   1672  CA  THR  222      29.375  49.277  19.939  1.00 24.06
ATOM   1673  CB  THR  222      30.893  49.423  19.960  1.00 24.59
ATOM   1674  OG1 THR  222      31.377  49.051  21.258  1.00 26.00
ATOM   1675  CG2 THR  222      31.299  50.860  19.640  1.00 24.67
ATOM   1676  C   THR  222      28.888  49.530  18.533  1.00 24.09
ATOM   1677  O   THR  222      28.248  50.530  18.259  1.00 24.72
ATOM   1678  N   GLY  223      29.211  48.597  17.646  1.00 24.40
ATOM   1679  CA  GLY  223      28.790  48.686  16.262  1.00 24.65
ATOM   1680  C   GLY  223      27.797  47.560  16.020  1.00 25.05
ATOM   1681  O   GLY  223      27.478  46.779  16.936  1.00 25.80
ATOM   1682  N   CYS  224      27.298  47.453  14.798  1.00 24.73
ATOM   1683  CA  CYS  224      26.338  46.405  14.504  1.00 24.18
ATOM   1684  CB  CYS  224      24.928  46.958  14.682  1.00 24.47
ATOM   1685  SG  CYS  224      23.640  45.925  13.998  1.00 25.11
ATOM   1686  C   CYS  224      26.550  45.895  13.085  1.00 23.65
ATOM   1687  O   CYS  224      26.618  46.683  12.144  1.00 24.07
ATOM   1688  N   ASN  225      26.650  44.578  12.941  1.00 23.06
ATOM   1689  CA  ASN  225      26.883  43.963  11.638  1.00 23.27
ATOM   1690  CB  ASN  225      28.346  44.230  11.210  1.00 26.15
ATOM   1691  CG  ASN  225      28.831  43.296  10.098  1.00 27.94
ATOM   1692  OD1 ASN  225      28.271  43.265   8.997  1.00 29.23
ATOM   1693  ND2 ASN  225      29.878  42.524  10.393  1.00 28.62
ATOM   1694  C   ASN  225      26.603  42.459  11.740  1.00 21.80
ATOM   1695  O   ASN  225      26.291  41.954  12.827  1.00 20.54
ATOM   1696  N   ALA  226      26.709  41.759  10.610  1.00 19.99
ATOM   1697  CA  ALA  226      26.478  40.322  10.566  1.00 19.47
ATOM   1698  CB  ALA  226      24.994  40.032  10.443  1.00 20.99
ATOM   1699  C   ALA  226      27.194  39.723   9.378  1.00 18.72
ATOM   1700  O   ALA  226      27.529  40.428   8.415  1.00 17.97
ATOM   1701  N   CYS  227      27.404  38.415   9.439  1.00 18.36
ATOM   1702  CA  CYS  227      28.077  37.675   8.368  1.00 19.35
ATOM   1703  CB  CYS  227      29.523  37.396   8.751  1.00 18.42
ATOM   1704  SG  CYS  227      29.556  36.326  10.207  1.00 20.13
ATOM   1705  C   CYS  227      27.331  36.352   8.291  1.00 19.81
ATOM   1706  O   CYS  227      26.702  35.951   9.280  1.00 20.62
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FIG. 4DD

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ATOM   1707  N   TYR  228      27.402  35.668   7.148  1.00 20.49
ATOM   1708  CA  TYR  228      26.705  34.384   6.989  1.00 20.56
ATOM   1709  CB  TYR  228      25.242  34.633   6.624  1.00 17.90
ATOM   1710  CG  TYR  228      25.096  35.134   5.204  1.00 15.65
ATOM   1711  CD1 TYR  228      24.922  34.249   4.145  1.00 15.81
ATOM   1712  CE1 TYR  228      24.885  34.701   2.823  1.00 15.89
ATOM   1713  CD2 TYR  228      25.221  36.483   4.913  1.00 15.28
ATOM   1714  CE2 TYR  228      25.186  36.949   3.601  1.00 16.08
ATOM   1715  CZ  TYR  228      25.022  36.051   2.564  1.00 16.76
ATOM   1716  OH  TYR  228      25.033  36.505   1.263  1.00 18.93
ATOM   1717  C   TYR  228      27.345  33.539   5.887  1.00 22.19
ATOM   1718  O   TYR  228      28.174  34.024   5.112  1.00 21.49
ATOM   1719  N   MSE  229      26.928  32.278   5.808  1.00 24.74
ATOM   1720  CA  MSE  229      27.438  31.349   4.808  1.00 26.69
ATOM   1721  CB  MSE  229      27.342  29.918   5.339  1.00 28.61
ATOM   1722  CG  MSE  229      28.167  29.637   6.598  1.00 32.37
ATOM   1723  SE  MSE  229      29.987  30.056   6.460  1.00 41.17
ATOM   1724  CE  MSE  229      30.544  28.874   5.098  1.00 36.30
ATOM   1725  C   MSE  229      26.663  31.470   3.481  1.00 27.83
ATOM   1726  O   MSE  229      25.535  30.994   3.363  1.00 28.02
ATOM   1727  N   GLU  230      27.282  32.109   2.492  1.00 29.19
ATOM   1728  CA  GLU  230      26.688  32.296   1.172  1.00 29.81
ATOM   1729  CB  GLU  230      27.165  33.623   0.577  1.00 30.83
ATOM   1730  CG  GLU  230      26.685  33.922  -0.843  1.00 32.33
ATOM   1731  CD  GLU  230      25.173  33.825  -0.989  1.00 34.04
ATOM   1732  OE1 GLU  230      24.663  32.698  -1.222  1.00 34.43
ATOM   1733  OE2 GLU  230      24.497  34.878  -0.858  1.00 33.65
ATOM   1734  C   GLU  230      27.127  31.143   0.282  1.00 30.91
ATOM   1735  O   GLU  230      27.958  30.319   0.685  1.00 30.80
ATOM   1736  N   GLU  231      26.562  31.078  -0.923  1.00 32.47
ATOM   1737  CA  GLU  231      26.885  30.024  -1.883  1.00 34.04
ATOM   1738  CB  GLU  231      25.668  29.696  -2.745  1.00 34.21
ATOM   1739  CG  GLU  231      24.408  29.396  -1.979  1.00 34.89
ATOM   1740  CD  GLU  231      24.452  28.054  -1.296  1.00 36.36
ATOM   1741  OE1 GLU  231      24.745  27.064  -2.002  1.00 36.80
ATOM   1742  OE2 GLU  231      24.182  27.981  -0.067  1.00 36.72
ATOM   1743  C   GLU  231      27.997  30.550  -2.777  1.00 35.65
ATOM   1744  O   GLU  231      27.889  31.663  -3.304  1.00 35.42
ATOM   1745  N   MSE  232      29.060  29.758  -2.952  1.00 37.13
ATOM   1746  CA  MSE  232      30.188  30.181  -3.780  1.00 38.19
ATOM   1747  CB  MSE  232      31.191  29.036  -3.935  1.00 41.27
ATOM   1748  CG  MSE  232      32.195  28.912  -2.765  1.00 45.40
ATOM   1749  SE  MSE  232      33.237  30.431  -2.467  1.00 52.07
ATOM   1750  CE  MSE  232      34.286  30.483  -3.969  1.00 48.20
ATOM   1751  C   MSE  232      29.694  30.664  -5.137  1.00 38.02
ATOM   1752  O   MSE  232      30.179  31.656  -5.678  1.00 36.84
ATOM   1753  N   GLN  233      28.698  29.970  -5.668  1.00 38.35
ATOM   1754  CA  GLN  233      28.110  30.331  -6.948  1.00 38.79
ATOM   1755  CB  GLN  233      26.954  29.373  -7.257  1.00 40.19
ATOM   1756  CG  GLN  233      25.658  30.041  -7.672  1.00 41.80
ATOM   1757  CD  GLN  233      24.460  29.119  -7.510  1.00 43.22
ATOM   1758  OE1 GLN  233      24.226  28.582  -6.424  1.00 44.27
ATOM   1759  NE2 GLN  233      23.688  28.936  -8.586  1.00 43.87
ATOM   1760  C   GLN  233      27.615  31.777  -6.936  1.00 38.45
ATOM   1761  O   GLN  233      27.495  32.407  -7.984  1.00 39.07
ATOM   1762  N   ASN  234      27.329  32.313  -5.753  1.00 37.79
ATOM   1763  CA  ASN  234      26.840  33.687  -5.668  1.00 36.56
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FIG. 4EE

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ATOM   1764  CB  ASN   234      25.657  33.771  -4.706  1.00 37.03
ATOM   1765  CG  ASN   234      24.505  32.864  -5.119  1.00 36.83
ATOM   1766  OD1 ASN   234      24.152  32.793  -6.299  1.00 36.50
ATOM   1767  ND2 ASN   234      23.910  32.173  -4.146  1.00 36.25
ATOM   1768  C   ASN   234      27.919  34.676  -5.250  1.00 35.71
ATOM   1769  O   ASN   234      27.712  35.890  -5.301  1.00 35.11
ATOM   1770  N   VAL   235      29.069  34.156  -4.837  1.00 35.22
ATOM   1771  CA  VAL   235      30.177  35.009  -4.439  1.00 34.85
ATOM   1772  CB  VAL   235      31.056  34.321  -3.384  1.00 34.01
ATOM   1773  CG1 VAL   235      31.949  35.343  -2.717  1.00 32.35
ATOM   1774  CG2 VAL   235      30.185  33.576  -2.376  1.00 32.63
ATOM   1775  C   VAL   235      30.999  35.209  -5.706  1.00 35.79
ATOM   1776  O   VAL   235      32.011  34.548  -5.910  1.00 35.65
ATOM   1777  N   GLU   236      30.556  36.125  -6.556  1.00 37.55
ATOM   1778  CA  GLU   236      31.220  36.383  -7.830  1.00 39.52
ATOM   1779  CB  GLU   236      30.337  37.284  -8.701  1.00 39.67
ATOM   1780  CG  GLU   236      29.242  36.539  -9.448  1.00 41.02
ATOM   1781  CD  GLU   236      28.214  37.467 -10.072  1.00 42.58
ATOM   1782  OE1 GLU   236      28.607  38.529 -10.630  1.00 42.67
ATOM   1783  OE2 GLU   236      27.009  37.121 -10.011  1.00 43.02
ATOM   1784  C   GLU   236      32.631  36.961  -7.782  1.00 40.97
ATOM   1785  O   GLU   236      33.328  36.967  -8.803  1.00 42.27
ATOM   1786  N   LEU   237      33.064  37.457  -6.628  1.00 41.32
ATOM   1787  CA  LEU   237      34.408  38.017  -6.538  1.00 41.63
ATOM   1788  CB  LEU   237      34.438  39.163  -5.537  1.00 41.68
ATOM   1789  CG  LEU   237      33.545  40.367  -5.820  1.00 42.50
ATOM   1790  CD1 LEU   237      33.630  41.301  -4.623  1.00 44.17
ATOM   1791  CD2 LEU   237      33.984  41.101  -7.085  1.00 42.46
ATOM   1792  C   LEU   237      35.454  36.970  -6.148  1.00 42.43
ATOM   1793  O   LEU   237      36.636  37.294  -6.010  1.00 42.30
ATOM   1794  N   VAL   238      35.019  35.724  -5.967  1.00 42.96
ATOM   1795  CA  VAL   238      35.922  34.629  -5.606  1.00 43.89
ATOM   1796  CB  VAL   238      35.917  34.380  -4.097  1.00 42.33
ATOM   1797  CG1 VAL   238      36.722  33.136  -3.769  1.00 41.32
ATOM   1798  CG2 VAL   238      36.503  35.578  -3.385  1.00 42.74
ATOM   1799  C   VAL   238      35.520  33.337  -6.313  1.00 45.65
ATOM   1800  O   VAL   238      34.755  32.555  -5.770  1.00 46.15
ATOM   1801  N   GLU   239      36.069  33.116  -7.510  1.00 47.60
ATOM   1802  CA  GLU   239      35.769  31.947  -8.346  1.00 48.96
ATOM   1803  CB  GLU   239      36.819  31.793  -9.448  1.00 51.17
ATOM   1804  CG  GLU   239      37.000  33.026 -10.290  1.00 53.95
ATOM   1805  CD  GLU   239      37.817  34.066  -9.570  1.00 56.27
ATOM   1806  OE1 GLU   239      39.070  33.982  -9.637  1.00 58.40
ATOM   1807  OE2 GLU   239      37.211  34.950  -8.918  1.00 57.25
ATOM   1808  C   GLU   239      35.599  30.594  -7.675  1.00 48.87
ATOM   1809  O   GLU   239      36.272  30.274  -6.701  1.00 48.25
ATOM   1810  N   GLY   240      34.705  29.797  -8.252  1.00 49.09
ATOM   1811  CA  GLY   240      34.412  28.469  -7.750  1.00 50.05
ATOM   1812  C   GLY   240      32.967  28.418  -7.296  1.00 51.04
ATOM   1813  O   GLY   240      32.482  29.379  -6.712  1.00 52.00
ATOM   1814  N   ASP   241      32.259  27.332  -7.580  1.00 51.38
ATOM   1815  CA  ASP   241      30.882  27.214  -7.127  1.00 52.10
ATOM   1816  CB  ASP   241      29.963  26.766  -8.252  1.00 52.95
ATOM   1817  CG  ASP   241      30.186  27.534  -9.529  1.00 53.84
ATOM   1818  OD1 ASP   241      30.046  28.779  -9.522  1.00 53.20
ATOM   1819  OD2 ASP   241      30.496  26.875 -10.546  1.00 53.97
ATOM   1820  C   ASP   241      30.924  26.122  -6.083  1.00 52.90
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FIG. 4FF

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ATOM   1821  O   ASP  241      29.898  25.563  -5.701  1.00 53.59
ATOM   1822  N   GLU  242      32.131  25.816  -5.626  1.00 53.45
ATOM   1823  CA  GLU  242      32.325  24.760  -4.646  1.00 53.65
ATOM   1824  CB  GLU  242      33.785  24.299  -4.670  1.00 55.19
ATOM   1825  CG  GLU  242      34.056  23.062  -3.826  1.00 57.57
ATOM   1826  CD  GLU  242      35.527  22.672  -3.811  1.00 58.85
ATOM   1827  OE1 GLU  242      36.063  22.340  -4.893  1.00 59.63
ATOM   1828  OE2 GLU  242      36.143  22.701  -2.717  1.00 59.85
ATOM   1829  C   GLU  242      31.933  25.159  -3.229  1.00 52.66
ATOM   1830  O   GLU  242      32.469  26.113  -2.661  1.00 53.15
ATOM   1831  N   GLY  243      30.987  24.418  -2.665  1.00 51.11
ATOM   1832  CA  GLY  243      30.545  24.673  -1.305  1.00 48.74
ATOM   1833  C   GLY  243      30.200  26.110  -0.967  1.00 46.87
ATOM   1834  O   GLY  243      29.879  26.917  -1.850  1.00 46.49
ATOM   1835  N   ARG  244      30.288  26.421   0.326  1.00 44.89
ATOM   1836  CA  ARG  244      29.967  27.748   0.838  1.00 43.27
ATOM   1837  CB  ARG  244      28.852  27.639   1.873  1.00 42.24
ATOM   1838  CG  ARG  244      27.571  27.040   1.339  1.00 42.16
ATOM   1839  CD  ARG  244      26.442  27.153   2.356  1.00 41.35
ATOM   1840  NE  ARG  244      25.254  26.425   1.925  1.00 39.30
ATOM   1841  CZ  ARG  244      24.702  25.446   2.630  1.00 39.15
ATOM   1842  NH1 ARG  244      25.236  25.085   3.794  1.00 38.10
ATOM   1843  NH2 ARG  244      23.627  24.821   2.168  1.00 38.77
ATOM   1844  C   ARG  244      31.121  28.524   1.465  1.00 42.34
ATOM   1845  O   ARG  244      32.089  27.945   1.958  1.00 41.77
ATOM   1846  N   MSE  245      30.990  29.849   1.446  1.00 42.07
ATOM   1847  CA  MSE  245      31.977  30.745   2.042  1.00 41.32
ATOM   1848  CB  MSE  245      32.846  31.391   0.974  1.00 42.25
ATOM   1849  CG  MSE  245      33.870  32.345   1.566  1.00 44.07
ATOM   1850  SE  MSE  245      34.884  33.206   0.332  1.00 47.16
ATOM   1851  CE  MSE  245      36.149  31.909  -0.005  1.00 44.40
ATOM   1852  C   MSE  245      31.324  31.863   2.863  1.00 40.37
ATOM   1853  O   MSE  245      30.525  32.644   2.338  1.00 40.13
ATOM   1854  N   CYS  246      31.664  31.940   4.148  1.00 38.95
ATOM   1855  CA  CYS  246      31.125  32.990   5.001  1.00 37.00
ATOM   1856  CB  CYS  246      31.794  32.953   6.376  1.00 37.69
ATOM   1857  SG  CYS  246      31.231  34.229   7.567  1.00 38.96
ATOM   1858  C   CYS  246      31.422  34.320   4.311  1.00 35.82
ATOM   1859  O   CYS  246      32.484  34.497   3.706  1.00 34.54
ATOM   1860  N   VAL  247      30.466  35.240   4.388  1.00 34.51
ATOM   1861  CA  VAL  247      30.591  36.566   3.782  1.00 32.46
ATOM   1862  CB  VAL  247      29.609  36.751   2.588  1.00 32.34
ATOM   1863  CG1 VAL  247      29.709  38.170   2.038  1.00 31.78
ATOM   1864  CG2 VAL  247      29.930  35.750   1.486  1.00 32.04
ATOM   1865  C   VAL  247      30.239  37.580   4.863  1.00 32.03
ATOM   1866  O   VAL  247      29.291  37.377   5.628  1.00 33.28
ATOM   1867  N   ASN  248      31.011  38.657   4.931  1.00 29.34
ATOM   1868  CA  ASN  248      30.792  39.699   5.917  1.00 27.36
ATOM   1869  CB  ASN  248      32.147  40.219   6.401  1.00 28.42
ATOM   1870  CG  ASN  248      32.031  41.471   7.253  1.00 29.34
ATOM   1871  OD1 ASN  248      30.975  41.774   7.816  1.00 29.82
ATOM   1872  ND2 ASN  248      33.141  42.201   7.374  1.00 29.54
ATOM   1873  C   ASN  248      29.983  40.798   5.257  1.00 27.10
ATOM   1874  O   ASN  248      30.531  41.618   4.503  1.00 26.98
ATOM   1875  N   THR  249      28.679  40.823   5.544  1.00 26.01
ATOM   1876  CA  THR  249      27.778  41.809   4.937  1.00 23.85
ATOM   1877  CB  THR  249      26.325  41.634   5.424  1.00 23.81
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FIG. 4GG

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ATOM   1878  OG1 THR   249      26.228  42.100   6.775  1.00 25.10
ATOM   1879  CG2 THR   249      25.899  40.156   5.380  1.00 22.15
ATOM   1880  C   THR   249      28.208  43.226   5.270  1.00 24.20
ATOM   1881  O   THR   249      28.023  44.143   4.467  1.00 23.38
ATOM   1882  N   GLU   250      28.777  43.406   6.462  1.00 24.31
ATOM   1883  CA  GLU   250      29.219  44.733   6.891  1.00 23.61
ATOM   1884  CB  GLU   250      30.446  45.145   6.060  1.00 23.87
ATOM   1885  CG  GLU   250      31.242  46.362   6.571  1.00 25.94
ATOM   1886  CD  GLU   250      32.237  46.041   7.700  1.00 25.83
ATOM   1887  OE1 GLU   250      32.728  44.893   7.813  1.00 25.67
ATOM   1888  OE2 GLU   250      32.552  46.960   8.473  1.00 26.46
ATOM   1889  C   GLU   250      28.003  45.624   6.589  1.00 23.30
ATOM   1890  O   GLU   250      28.110  46.648   5.896  1.00 23.33
ATOM   1891  N   TRP   251      26.841  45.208   7.096  1.00 22.28
ATOM   1892  CA  TRP   251      25.609  45.940   6.840  1.00 22.36
ATOM   1893  CB  TRP   251      24.376  45.077   7.133  1.00 20.65
ATOM   1894  CG  TRP   251      24.133  44.726   8.543  1.00 18.29
ATOM   1895  CD2 TRP   251      23.308  43.648   9.016  1.00 16.51
ATOM   1896  CE2 TRP   251      23.279  43.725  10.424  1.00 15.08
ATOM   1897  CE3 TRP   251      22.589  42.635   8.384  1.00 16.17
ATOM   1898  CD1 TRP   251      24.565  45.395   9.652  1.00 17.71
ATOM   1899  NE1 TRP   251      24.051  44.795  10.795  1.00 17.10
ATOM   1900  CZ2 TRP   251      22.567  42.830  11.201  1.00 14.23
ATOM   1901  CZ3 TRP   251      21.872  41.737   9.171  1.00 15.72
ATOM   1902  CH2 TRP   251      21.869  41.842  10.559  1.00 14.23
ATOM   1903  C   TRP   251      25.445  47.283   7.523  1.00 23.49
ATOM   1904  O   TRP   251      24.541  48.044   7.167  1.00 23.95
ATOM   1905  N   GLY   252      26.302  47.579   8.500  1.00 24.44
ATOM   1906  CA  GLY   252      26.214  48.857   9.179  1.00 25.17
ATOM   1907  C   GLY   252      26.195  49.979   8.152  1.00 26.19
ATOM   1908  O   GLY   252      25.715  51.086   8.429  1.00 26.19
ATOM   1909  N   ALA   253      26.714  49.675   6.960  1.00 26.83
ATOM   1910  CA  ALA   253      26.791  50.622   5.851  1.00 27.86
ATOM   1911  CB  ALA   253      27.822  50.148   4.851  1.00 27.90
ATOM   1912  C   ALA   253      25.448  50.834   5.144  1.00 28.52
ATOM   1913  O   ALA   253      25.249  51.834   4.448  1.00 27.73
ATOM   1914  N   PHE   254      24.536  49.884   5.314  1.00 30.23
ATOM   1915  CA  PHE   254      23.224  49.974   4.696  1.00 31.42
ATOM   1916  CB  PHE   254      22.289  48.947   5.314  1.00 31.71
ATOM   1917  CG  PHE   254      20.899  48.995   4.768  1.00 31.90
ATOM   1918  CD1 PHE   254      20.655  48.736   3.429  1.00 31.47
ATOM   1919  CD2 PHE   254      19.824  49.273   5.600  1.00 32.95
ATOM   1920  CE1 PHE   254      19.367  48.746   2.927  1.00 31.38
ATOM   1921  CE2 PHE   254      18.518  49.285   5.096  1.00 32.69
ATOM   1922  CZ  PHE   254      18.295  49.021   3.763  1.00 31.47
ATOM   1923  C   PHE   254      22.664  51.367   4.928  1.00 32.56
ATOM   1924  O   PHE   254      22.638  51.839   6.064  1.00 33.19
ATOM   1925  N   GLY   255      22.227  52.017   3.849  1.00 33.62
ATOM   1926  CA  GLY   255      21.674  53.354   3.947  1.00 34.98
ATOM   1927  C   GLY   255      22.673  54.429   3.565  1.00 36.85
ATOM   1928  O   GLY   255      22.317  55.604   3.424  1.00 36.70
ATOM   1929  N   ASP   256      23.932  54.038   3.395  1.00 38.95
ATOM   1930  CA  ASP   256      24.966  55.000   3.038  1.00 41.47
ATOM   1931  CB  ASP   256      26.349  54.347   3.088  1.00 41.77
ATOM   1932  CG  ASP   256      26.880  54.224   4.502  1.00 42.36
ATOM   1933  OD1 ASP   256      26.573  55.120   5.322  1.00 43.08
ATOM   1934  OD2 ASP   256      27.617  53.251   4.791  1.00 42.28
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FIG. 4HH

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ATOM   1935  C   ASP  256      24.744  55.636   1.666  1.00 43.10
ATOM   1936  O   ASP  256      25.489  56.533   1.261  1.00 44.08
ATOM   1937  N   SER  257      23.729  55.171   0.946  1.00 44.19
ATOM   1938  CA  SER  257      23.427  55.738  -0.363  1.00 45.32
ATOM   1939  CB  SER  257      23.714  54.713  -1.467  1.00 45.78
ATOM   1940  OG  SER  257      22.845  53.601  -1.375  1.00 46.48
ATOM   1941  C   SER  257      21.967  56.204  -0.423  1.00 45.41
ATOM   1942  O   SER  257      21.378  56.316  -1.501  1.00 46.14
ATOM   1943  N   GLY  258      21.393  56.466   0.751  1.00 45.52
ATOM   1944  CA  GLY  258      20.018  56.933   0.835  1.00 45.22
ATOM   1945  C   GLY  258      18.922  55.896   1.042  1.00 45.11
ATOM   1946  O   GLY  258      17.745  56.253   1.068  1.00 45.45
ATOM   1947  N   GLU  259      19.284  54.627   1.205  1.00 44.67
ATOM   1948  CA  GLU  259      18.288  53.572   1.380  1.00 44.04
ATOM   1949  CB  GLU  259      18.954  52.187   1.415  1.00 44.23
ATOM   1950  CG  GLU  259      19.952  51.916   0.295  1.00 44.88
ATOM   1951  CD  GLU  259      21.318  52.552   0.548  1.00 45.53
ATOM   1952  OE1 GLU  259      21.381  53.785   0.753  1.00 44.98
ATOM   1953  OE2 GLU  259      22.335  51.817   0.537  1.00 45.95
ATOM   1954  C   GLU  259      17.462  53.749   2.647  1.00 43.91
ATOM   1955  O   GLU  259      16.461  53.061   2.836  1.00 43.49
ATOM   1956  N   LEU  260      17.875  54.661   3.520  1.00 43.87
ATOM   1957  CA  LEU  260      17.143  54.865   4.765  1.00 44.40
ATOM   1958  CB  LEU  260      18.023  54.513   5.967  1.00 44.36
ATOM   1959  CG  LEU  260      18.398  53.041   6.153  1.00 44.87
ATOM   1960  CD1 LEU  260      19.315  52.879   7.369  1.00 44.30
ATOM   1961  CD2 LEU  260      17.127  52.216   6.307  1.00 44.88
ATOM   1962  C   LEU  260      16.632  56.282   4.932  1.00 44.59
ATOM   1963  O   LEU  260      15.744  56.534   5.749  1.00 44.72
ATOM   1964  N   ASP  261      17.200  57.202   4.161  1.00 44.48
ATOM   1965  CA  ASP  261      16.821  58.608   4.234  1.00 44.18
ATOM   1966  CB  ASP  261      16.813  59.224   2.841  1.00 44.99
ATOM   1967  CG  ASP  261      18.192  59.310   2.247  1.00 46.23
ATOM   1968  OD1 ASP  261      19.165  58.994   2.980  1.00 46.42
ATOM   1969  OD2 ASP  261      18.296  59.697   1.055  1.00 46.79
ATOM   1970  C   ASP  261      15.482  58.885   4.892  1.00 43.00
ATOM   1971  O   ASP  261      15.415  59.592   5.898  1.00 42.63
ATOM   1972  N   GLU  262      14.424  58.317   4.320  1.00 41.88
ATOM   1973  CA  GLU  262      13.070  58.525   4.810  1.00 41.00
ATOM   1974  CB  GLU  262      12.088  57.744   3.940  1.00 41.65
ATOM   1975  CG  GLU  262      12.249  56.254   3.999  1.00 43.54
ATOM   1976  CD  GLU  262      11.359  55.562   2.996  1.00 45.44
ATOM   1977  OE1 GLU  262      11.715  55.561   1.800  1.00 47.21
ATOM   1978  OE2 GLU  262      10.296  55.031   3.391  1.00 47.29
ATOM   1979  C   GLU  262      12.830  58.211   6.286  1.00 39.99
ATOM   1980  O   GLU  262      11.997  58.852   6.918  1.00 40.22
ATOM   1981  N   PHE  263      13.545  57.238   6.845  1.00 38.83
ATOM   1982  CA  PHE  263      13.360  56.908   8.258  1.00 37.00
ATOM   1983  CB  PHE  263      13.684  55.430   8.512  1.00 34.37
ATOM   1984  CG  PHE  263      12.828  54.476   7.717  1.00 32.41
ATOM   1985  CD1 PHE  263      13.366  53.753   6.660  1.00 30.67
ATOM   1986  CD2 PHE  263      11.474  54.317   8.012  1.00 30.95
ATOM   1987  CE1 PHE  263      12.567  52.886   5.909  1.00 29.82
ATOM   1988  CE2 PHE  263      10.667  53.450   7.261  1.00 28.87
ATOM   1989  CZ  PHE  263      11.214  52.737   6.213  1.00 29.09
ATOM   1990  C   PHE  263      14.197  57.797   9.190  1.00 36.78
ATOM   1991  O   PHE  263      13.809  58.041  10.327  1.00 37.58
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FIG. 4II

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ATOM   1992  N   LEU  264      15.328  58.301   8.712  1.00 36.72
ATOM   1993  CA  LEU  264      16.193  59.142   9.542  1.00 37.11
ATOM   1994  CB  LEU  264      17.389  59.638   8.725  1.00 36.98
ATOM   1995  CG  LEU  264      18.131  58.621   7.852  1.00 36.59
ATOM   1996  CD1 LEU  264      19.233  59.346   7.077  1.00 35.39
ATOM   1997  CD2 LEU  264      18.701  57.503   8.717  1.00 35.46
ATOM   1998  C   LEU  264      15.482  60.350  10.158  1.00 37.28
ATOM   1999  O   LEU  264      14.879  61.148   9.451  1.00 38.03
ATOM   2000  N   LEU  265      15.574  60.480  11.479  1.00 37.63
ATOM   2001  CA  LEU  265      14.965  61.585  12.215  1.00 37.33
ATOM   2002  CB  LEU  265      14.380  61.070  13.527  1.00 36.25
ATOM   2003  CG  LEU  265      13.529  59.807  13.417  1.00 35.76
ATOM   2004  CD1 LEU  265      13.157  59.295  14.808  1.00 35.17
ATOM   2005  CD2 LEU  265      12.292  60.120  12.598  1.00 35.59
ATOM   2006  C   LEU  265      16.054  62.613  12.521  1.00 38.22
ATOM   2007  O   LEU  265      17.239  62.285  12.486  1.00 38.34
ATOM   2008  N   GLU  266      15.653  63.844  12.832  1.00 39.22
ATOM   2009  CA  GLU  266      16.599  64.922  13.137  1.00 40.56
ATOM   2010  CB  GLU  266      15.874  66.101  13.813  1.00 41.82
ATOM   2011  CG  GLU  266      15.277  65.777  15.196  1.00 44.28
ATOM   2012  CD  GLU  266      14.612  66.974  15.886  1.00 44.95
ATOM   2013  OE1 GLU  266      13.543  67.432  15.410  1.00 45.08
ATOM   2014  OE2 GLU  266      15.163  67.452  16.910  1.00 45.53
ATOM   2015  C   GLU  266      17.733  64.435  14.036  1.00 40.54
ATOM   2016  O   GLU  266      18.910  64.657  13.750  1.00 40.69
ATOM   2017  N   TYR  267      17.366  63.760  15.121  1.00 40.61
ATOM   2018  CA  TYR  267      18.342  63.234  16.062  1.00 40.30
ATOM   2019  CB  TYR  267      17.639  62.364  17.110  1.00 39.44
ATOM   2020  CG  TYR  267      16.216  62.784  17.423  1.00 38.98
ATOM   2021  CD1 TYR  267      15.134  61.967  17.066  1.00 38.66
ATOM   2022  CE1 TYR  267      13.813  62.342  17.349  1.00 38.28
ATOM   2023  CD2 TYR  267      15.943  63.995  18.075  1.00 38.72
ATOM   2024  CE2 TYR  267      14.619  64.381  18.364  1.00 38.45
ATOM   2025  CZ  TYR  267      13.564  63.548  17.996  1.00 38.30
ATOM   2026  OH  TYR  267      12.267  63.923  18.251  1.00 37.22
ATOM   2027  C   TYR  267      19.381  62.403  15.296  1.00 40.27
ATOM   2028  O   TYR  267      20.580  62.469  15.579  1.00 40.14
ATOM   2029  N   ASP  268      18.909  61.626  14.324  1.00 40.61
ATOM   2030  CA  ASP  268      19.781  60.790  13.511  1.00 40.87
ATOM   2031  CB  ASP  268      18.946  59.920  12.566  1.00 39.36
ATOM   2032  CG  ASP  268      18.183  58.843  13.301  1.00 38.52
ATOM   2033  OD1 ASP  268      18.819  58.118  14.082  1.00 39.79
ATOM   2034  OD2 ASP  268      16.961  58.711  13.110  1.00 36.13
ATOM   2035  C   ASP  268      20.764  61.643  12.712  1.00 41.97
ATOM   2036  O   ASP  268      21.956  61.339  12.667  1.00 42.91
ATOM   2037  N   ARG  269      20.266  62.710  12.090  1.00 42.73
ATOM   2038  CA  ARG  269      21.113  63.606  11.310  1.00 43.23
ATOM   2039  CB  ARG  269      20.302  64.793  10.786  1.00 45.34
ATOM   2040  CG  ARG  269      18.923  64.464  10.223  1.00 47.46
ATOM   2041  CD  ARG  269      19.000  63.819   8.864  1.00 49.22
ATOM   2042  NE  ARG  269      17.667  63.552   8.337  1.00 52.67
ATOM   2043  CZ  ARG  269      17.426  62.969   7.165  1.00 54.63
ATOM   2044  NH1 ARG  269      18.436  62.591   6.386  1.00 55.41
ATOM   2045  NH2 ARG  269      16.173  62.747   6.775  1.00 55.38
ATOM   2046  C   ARG  269      22.204  64.150  12.231  1.00 42.99
ATOM   2047  O   ARG  269      23.400  63.999  11.977  1.00 43.63
ATOM   2048  N   LEU  270      21.777  64.796  13.305  1.00 41.99
```

FIG. 4JJ

ATOM	2049	CA	LEU	270	22.702	65.372	14.261	1.00	41.33
ATOM	2050	CB	LEU	270	21.924	65.812	15.502	1.00	41.15
ATOM	2051	CG	LEU	270	21.004	67.002	15.217	1.00	40.34
ATOM	2052	CD1	LEU	270	19.964	67.182	16.307	1.00	39.94
ATOM	2053	CD2	LEU	270	21.879	68.237	15.084	1.00	40.26
ATOM	2054	C	LEU	270	23.828	64.406	14.635	1.00	41.26
ATOM	2055	O	LEU	270	25.009	64.762	14.553	1.00	41.76
ATOM	2056	N	VAL	271	23.462	63.188	15.030	1.00	40.24
ATOM	2057	CA	VAL	271	24.443	62.177	15.415	1.00	40.08
ATOM	2058	CB	VAL	271	23.776	60.838	15.730	1.00	40.42
ATOM	2059	CG1	VAL	271	24.846	59.800	16.050	1.00	39.86
ATOM	2060	CG2	VAL	271	22.796	61.000	16.891	1.00	40.86
ATOM	2061	C	VAL	271	25.477	61.903	14.329	1.00	40.51
ATOM	2062	O	VAL	271	26.676	61.832	14.595	1.00	40.15
ATOM	2063	N	ASP	272	24.998	61.730	13.103	1.00	40.78
ATOM	2064	CA	ASP	272	25.866	61.447	11.977	1.00	40.36
ATOM	2065	CB	ASP	272	25.038	61.344	10.695	1.00	39.16
ATOM	2066	CG	ASP	272	25.792	60.670	9.553	1.00	38.09
ATOM	2067	OD1	ASP	272	26.821	60.000	9.807	1.00	36.54
ATOM	2068	OD2	ASP	272	25.335	60.798	8.394	1.00	37.12
ATOM	2069	C	ASP	272	26.901	62.544	11.849	1.00	40.88
ATOM	2070	O	ASP	272	28.099	62.297	11.953	1.00	40.75
ATOM	2071	N	GLU	273	26.429	63.763	11.638	1.00	41.96
ATOM	2072	CA	GLU	273	27.321	64.896	11.477	1.00	43.14
ATOM	2073	CB	GLU	273	26.501	66.170	11.470	1.00	44.13
ATOM	2074	CG	GLU	273	25.576	66.214	10.272	1.00	46.73
ATOM	2075	CD	GLU	273	24.629	67.388	10.308	1.00	48.40
ATOM	2076	OE1	GLU	273	25.047	68.455	10.828	1.00	49.15
ATOM	2077	OE2	GLU	273	23.482	67.241	9.811	1.00	48.64
ATOM	2078	C	GLU	273	28.428	64.968	12.517	1.00	43.48
ATOM	2079	O	GLU	273	29.575	65.279	12.187	1.00	43.59
ATOM	2080	N	SER	274	28.095	64.666	13.767	1.00	44.05
ATOM	2081	CA	SER	274	29.089	64.702	14.837	1.00	44.54
ATOM	2082	CB	SER	274	28.421	64.568	16.205	1.00	45.39
ATOM	2083	OG	SER	274	27.496	65.611	16.424	1.00	48.14
ATOM	2084	C	SER	274	30.106	63.582	14.694	1.00	44.23
ATOM	2085	O	SER	274	31.292	63.783	14.931	1.00	44.76
ATOM	2086	N	SER	275	29.632	62.400	14.318	1.00	43.84
ATOM	2087	CA	SER	275	30.489	61.227	14.162	1.00	43.42
ATOM	2088	CB	SER	275	29.754	60.139	13.392	1.00	43.28
ATOM	2089	OG	SER	275	29.758	60.444	12.010	1.00	42.94
ATOM	2090	C	SER	275	31.789	61.535	13.426	1.00	43.34
ATOM	2091	O	SER	275	31.914	62.552	12.738	1.00	43.76
ATOM	2092	N	ALA	276	32.756	60.639	13.570	1.00	42.68
ATOM	2093	CA	ALA	276	34.034	60.805	12.906	1.00	42.98
ATOM	2094	CB	ALA	276	35.108	60.015	13.639	1.00	42.92
ATOM	2095	C	ALA	276	33.930	60.319	11.465	1.00	43.23
ATOM	2096	O	ALA	276	34.936	60.277	10.751	1.00	44.60
ATOM	2097	N	ASN	277	32.722	59.949	11.039	1.00	42.10
ATOM	2098	CA	ASN	277	32.517	59.447	9.691	1.00	40.87
ATOM	2099	CB	ASN	277	32.615	57.927	9.685	1.00	41.63
ATOM	2100	CG	ASN	277	31.654	57.283	10.659	1.00	42.64
ATOM	2101	OD1	ASN	277	30.670	57.898	11.067	1.00	43.50
ATOM	2102	ND2	ASN	277	31.925	56.033	11.029	1.00	42.98
ATOM	2103	C	ASN	277	31.178	59.865	9.104	1.00	40.57
ATOM	2104	O	ASN	277	30.430	59.039	8.579	1.00	39.89
ATOM	2105	N	PRO	278	30.868	61.163	9.163	1.00	40.83

FIG. 4KK

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ATOM   2106  CD  PRO   278      31.783  62.282   9.451  1.00 40.90
ATOM   2107  CA  PRO   278      29.600  61.657   8.623  1.00 40.71
ATOM   2108  CB  PRO   278      29.807  63.175   8.579  1.00 40.88
ATOM   2109  CG  PRO   278      31.303  63.326   8.474  1.00 41.27
ATOM   2110  C   PRO   278      29.239  61.074   7.258  1.00 40.60
ATOM   2111  O   PRO   278      29.949  61.284   6.270  1.00 40.71
ATOM   2112  N   GLY   279      28.131  60.338   7.216  1.00 40.34
ATOM   2113  CA  GLY   279      27.676  59.747   5.971  1.00 39.10
ATOM   2114  C   GLY   279      27.904  58.252   5.828  1.00 38.94
ATOM   2115  O   GLY   279      27.315  57.635   4.952  1.00 39.74
ATOM   2116  N   GLN   280      28.735  57.660   6.683  1.00 38.66
ATOM   2117  CA  GLN   280      29.049  56.230   6.605  1.00 37.75
ATOM   2118  CB  GLN   280      30.563  56.043   6.513  1.00 37.97
ATOM   2119  CG  GLN   280      31.243  56.954   5.509  1.00 39.85
ATOM   2120  CD  GLN   280      32.743  57.046   5.730  1.00 40.76
ATOM   2121  OE1 GLN   280      33.465  56.058   5.587  1.00 41.39
ATOM   2122  NE2 GLN   280      33.220  58.240   6.083  1.00 41.57
ATOM   2123  C   GLN   280      28.553  55.455   7.817  1.00 36.99
ATOM   2124  O   GLN   280      28.645  55.939   8.941  1.00 37.89
ATOM   2125  N   GLN   281      28.054  54.242   7.592  1.00 35.75
ATOM   2126  CA  GLN   281      27.572  53.401   8.681  1.00 34.04
ATOM   2127  CB  GLN   281      28.590  53.404   9.829  1.00 33.35
ATOM   2128  CG  GLN   281      29.971  52.951   9.447  1.00 33.09
ATOM   2129  CD  GLN   281      29.967  51.576   8.800  1.00 34.44
ATOM   2130  OE1 GLN   281      29.917  51.451   7.572  1.00 33.95
ATOM   2131  NE2 GLN   281      30.000  50.529   9.630  1.00 34.63
ATOM   2132  C   GLN   281      26.210  53.831   9.237  1.00 33.42
ATOM   2133  O   GLN   281      25.895  53.530  10.390  1.00 34.87
ATOM   2134  N   LEU   282      25.395  54.511   8.436  1.00 31.53
ATOM   2135  CA  LEU   282      24.098  54.992   8.913  1.00 29.87
ATOM   2136  CB  LEU   282      23.345  55.685   7.777  1.00 30.15
ATOM   2137  CG  LEU   282      24.030  56.871   7.085  1.00 30.41
ATOM   2138  CD1 LEU   282      22.963  57.741   6.435  1.00 29.82
ATOM   2139  CD2 LEU   282      24.815  57.699   8.097  1.00 30.66
ATOM   2140  C   LEU   282      23.191  53.949   9.578  1.00 28.70
ATOM   2141  O   LEU   282      22.716  54.153  10.698  1.00 28.78
ATOM   2142  N   TYR   283      22.935  52.841   8.894  1.00 27.35
ATOM   2143  CA  TYR   283      22.095  51.793   9.461  1.00 26.53
ATOM   2144  CB  TYR   283      22.233  50.511   8.633  1.00 24.41
ATOM   2145  CG  TYR   283      21.420  49.338   9.143  1.00 22.90
ATOM   2146  CD1 TYR   283      20.021  49.413   9.210  1.00 21.94
ATOM   2147  CE1 TYR   283      19.257  48.318   9.609  1.00 20.96
ATOM   2148  CD2 TYR   283      22.038  48.129   9.503  1.00 21.53
ATOM   2149  CE2 TYR   283      21.279  47.030   9.907  1.00 20.87
ATOM   2150  CZ  TYR   283      19.886  47.140   9.950  1.00 21.33
ATOM   2151  OH  TYR   283      19.105  46.068  10.310  1.00 23.85
ATOM   2152  C   TYR   283      22.567  51.532  10.891  1.00 27.12
ATOM   2153  O   TYR   283      21.783  51.521  11.841  1.00 28.95
ATOM   2154  N   GLU   284      23.869  51.352  11.035  1.00 26.60
ATOM   2155  CA  GLU   284      24.486  51.072  12.317  1.00 26.43
ATOM   2156  CB  GLU   284      25.982  50.905  12.108  1.00 27.03
ATOM   2157  CG  GLU   284      26.763  50.680  13.375  1.00 27.21
ATOM   2158  CD  GLU   284      28.224  50.492  13.082  1.00 27.57
ATOM   2159  OE1 GLU   284      28.897  51.506  12.734  1.00 27.02
ATOM   2160  OE2 GLU   284      28.670  49.319  13.185  1.00 26.30
ATOM   2161  C   GLU   284      24.249  52.133  13.381  1.00 26.81
ATOM   2162  O   GLU   284      24.197  51.826  14.582  1.00 26.06
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FIG. 4LL

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ATOM   2163  N   LYS  285      24.134  53.384  12.940  1.00 27.07
ATOM   2164  CA  LYS  285      23.926  54.502  13.860  1.00 27.39
ATOM   2165  CB  LYS  285      24.339  55.825  13.186  1.00 25.99
ATOM   2166  CG  LYS  285      25.840  56.012  13.132  1.00 24.13
ATOM   2167  CD  LYS  285      26.235  57.110  12.179  1.00 23.29
ATOM   2168  CE  LYS  285      27.755  57.193  12.052  1.00 22.03
ATOM   2169  NZ  LYS  285      28.142  58.198  11.027  1.00 21.72
ATOM   2170  C   LYS  285      22.488  54.595  14.368  1.00 28.05
ATOM   2171  O   LYS  285      22.086  55.615  14.941  1.00 28.61
ATOM   2172  N   LEU  286      21.717  53.535  14.144  1.00 27.60
ATOM   2173  CA  LEU  286      20.335  53.488  14.599  1.00 27.30
ATOM   2174  CB  LEU  286      19.399  53.157  13.435  1.00 28.57
ATOM   2175  CG  LEU  286      19.375  54.167  12.279  1.00 30.25
ATOM   2176  CD1 LEU  286      18.480  53.647  11.139  1.00 29.98
ATOM   2177  CD2 LEU  286      18.863  55.507  12.780  1.00 29.35
ATOM   2178  C   LEU  286      20.260  52.381  15.632  1.00 27.01
ATOM   2179  O   LEU  286      19.296  52.294  16.399  1.00 27.55
ATOM   2180  N   ILE  287      21.306  51.554  15.645  1.00 26.00
ATOM   2181  CA  ILE  287      21.415  50.399  16.532  1.00 24.38
ATOM   2182  CB  ILE  287      21.551  49.141  15.715  1.00 23.92
ATOM   2183  CG2 ILE  287      21.470  47.919  16.628  1.00 22.70
ATOM   2184  CG1 ILE  287      20.510  49.158  14.597  1.00 22.87
ATOM   2185  CD1 ILE  287      20.676  48.042  13.607  1.00 22.79
ATOM   2186  C   ILE  287      22.639  50.444  17.433  1.00 24.65
ATOM   2187  O   ILE  287      22.550  50.255  18.644  1.00 23.54
ATOM   2188  N   GLY  288      23.791  50.668  16.810  1.00 25.94
ATOM   2189  CA  GLY  288      25.060  50.714  17.519  1.00 26.86
ATOM   2190  C   GLY  288      25.081  51.266  18.927  1.00 27.76
ATOM   2191  O   GLY  288      24.697  52.412  19.164  1.00 28.19
ATOM   2192  N   GLY  289      25.554  50.445  19.860  1.00 28.95
ATOM   2193  CA  GLY  289      25.656  50.856  21.249  1.00 30.64
ATOM   2194  C   GLY  289      26.632  52.007  21.407  1.00 31.92
ATOM   2195  O   GLY  289      26.930  52.442  22.509  1.00 32.56
ATOM   2196  N   LYS  290      27.133  52.504  20.291  1.00 32.83
ATOM   2197  CA  LYS  290      28.067  53.607  20.296  1.00 33.99
ATOM   2198  CB  LYS  290      29.104  53.373  19.191  1.00 35.04
ATOM   2199  CG  LYS  290      29.858  54.598  18.665  1.00 36.71
ATOM   2200  CD  LYS  290      31.032  54.996  19.551  1.00 38.80
ATOM   2201  CE  LYS  290      31.936  56.011  18.839  1.00 39.77
ATOM   2202  NZ  LYS  290      32.864  56.707  19.787  1.00 41.04
ATOM   2203  C   LYS  290      27.278  54.880  20.035  1.00 34.58
ATOM   2204  O   LYS  290      27.810  55.984  20.138  1.00 35.79
ATOM   2205  N   TYR  291      26.001  54.734  19.708  1.00 33.80
ATOM   2206  CA  TYR  291      25.196  55.907  19.406  1.00 33.61
ATOM   2207  CB  TYR  291      25.010  56.046  17.892  1.00 33.22
ATOM   2208  CG  TYR  291      26.256  55.752  17.084  1.00 33.77
ATOM   2209  CD1 TYR  291      26.659  54.435  16.838  1.00 34.23
ATOM   2210  CE1 TYR  291      27.789  54.155  16.065  1.00 34.17
ATOM   2211  CD2 TYR  291      27.021  56.783  16.542  1.00 33.61
ATOM   2212  CE2 TYR  291      28.150  56.515  15.773  1.00 33.54
ATOM   2213  CZ  TYR  291      28.528  55.200  15.532  1.00 33.76
ATOM   2214  OH  TYR  291      29.620  54.928  14.729  1.00 34.36
ATOM   2215  C   TYR  291      23.836  55.874  20.070  1.00 33.11
ATOM   2216  O   TYR  291      23.069  56.828  19.975  1.00 32.86
ATOM   2217  N   MSE  292      23.521  54.778  20.737  1.00 33.27
ATOM   2218  CA  MSE  292      22.230  54.699  21.389  1.00 33.18
ATOM   2219  CB  MSE  292      22.066  53.349  22.062  1.00 33.77
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FIG. 4MM

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ATOM   2220  CG  MSE   292      20.639  52.975  22.314  1.00 35.15
ATOM   2221  SE  MSE   292      20.564  51.230  22.803  1.00 41.54
ATOM   2222  CE  MSE   292      20.269  50.385  21.171  1.00 35.91
ATOM   2223  C   MSE   292      22.148  55.818  22.423  1.00 32.97
ATOM   2224  O   MSE   292      21.227  56.637  22.400  1.00 33.49
ATOM   2225  N   GLY   293      23.131  55.861  23.315  1.00 32.96
ATOM   2226  CA  GLY   293      23.151  56.892  24.334  1.00 32.25
ATOM   2227  C   GLY   293      23.067  58.290  23.750  1.00 32.18
ATOM   2228  O   GLY   293      22.307  59.126  24.241  1.00 33.24
ATOM   2229  N   GLU   294      23.835  58.560  22.702  1.00 31.47
ATOM   2230  CA  GLU   294      23.809  59.883  22.096  1.00 31.38
ATOM   2231  CB  GLU   294      24.875  59.971  21.008  1.00 33.29
ATOM   2232  CG  GLU   294      24.986  61.321  20.304  1.00 34.67
ATOM   2233  CD  GLU   294      25.227  62.474  21.257  1.00 35.80
ATOM   2234  OE1 GLU   294      25.708  62.244  22.389  1.00 36.49
ATOM   2235  OE2 GLU   294      24.946  63.623  20.858  1.00 37.16
ATOM   2236  C   GLU   294      22.428  60.192  21.521  1.00 30.62
ATOM   2237  O   GLU   294      21.919  61.305  21.664  1.00 30.94
ATOM   2238  N   LEU   295      21.818  59.204  20.878  1.00 29.56
ATOM   2239  CA  LEU   295      20.495  59.392  20.303  1.00 29.24
ATOM   2240  CB  LEU   295      20.030  58.112  19.589  1.00 27.27
ATOM   2241  CG  LEU   295      20.389  58.007  18.099  1.00 25.46
ATOM   2242  CD1 LEU   295      19.979  56.668  17.522  1.00 21.87
ATOM   2243  CD2 LEU   295      19.677  59.136  17.352  1.00 25.71
ATOM   2244  C   LEU   295      19.497  59.787  21.388  1.00 29.98
ATOM   2245  O   LEU   295      18.587  60.573  21.156  1.00 30.19
ATOM   2246  N   VAL   296      19.665  59.250  22.585  1.00 31.23
ATOM   2247  CA  VAL   296      18.745  59.590  23.657  1.00 32.87
ATOM   2248  CB  VAL   296      18.890  58.623  24.831  1.00 32.48
ATOM   2249  CG1 VAL   296      17.827  58.899  25.868  1.00 32.99
ATOM   2250  CG2 VAL   296      18.762  57.198  24.323  1.00 33.56
ATOM   2251  C   VAL   296      19.020  61.025  24.122  1.00 33.74
ATOM   2252  O   VAL   296      18.086  61.778  24.431  1.00 33.68
ATOM   2253  N   ARG   297      20.296  61.409  24.145  1.00 34.02
ATOM   2254  CA  ARG   297      20.659  62.757  24.563  1.00 35.34
ATOM   2255  CB  ARG   297      22.147  63.008  24.342  1.00 34.89
ATOM   2256  CG  ARG   297      22.940  63.279  25.609  1.00 35.27
ATOM   2257  CD  ARG   297      23.791  64.525  25.454  1.00 35.98
ATOM   2258  NE  ARG   297      24.226  64.700  24.074  1.00 37.11
ATOM   2259  CZ  ARG   297      24.476  65.878  23.513  1.00 37.43
ATOM   2260  NH1 ARG   297      24.348  66.994  24.226  1.00 38.45
ATOM   2261  NH2 ARG   297      24.809  65.944  22.229  1.00 36.61
ATOM   2262  C   ARG   297      19.870  63.766  23.747  1.00 36.07
ATOM   2263  O   ARG   297      19.103  64.574  24.285  1.00 36.76
ATOM   2264  N   LEU   298      20.063  63.699  22.437  1.00 36.93
ATOM   2265  CA  LEU   298      19.407  64.596  21.500  1.00 37.55
ATOM   2266  CB  LEU   298      19.768  64.178  20.077  1.00 37.28
ATOM   2267  CG  LEU   298      21.272  64.065  19.816  1.00 36.13
ATOM   2268  CD1 LEU   298      21.478  63.784  18.341  1.00 36.85
ATOM   2269  CD2 LEU   298      21.991  65.356  20.218  1.00 35.02
ATOM   2270  C   LEU   298      17.892  64.633  21.670  1.00 38.53
ATOM   2271  O   LEU   298      17.276  65.708  21.618  1.00 38.44
ATOM   2272  N   VAL   299      17.289  63.462  21.866  1.00 39.23
ATOM   2273  CA  VAL   299      15.839  63.389  22.054  1.00 40.08
ATOM   2274  CB  VAL   299      15.349  61.932  22.110  1.00 39.44
ATOM   2275  CG1 VAL   299      13.844  61.892  22.385  1.00 37.91
ATOM   2276  CG2 VAL   299      15.676  61.240  20.802  1.00 38.72
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FIG. 4NN

ATOM	2277	C	VAL	299	15.435	64.087	23.350	1.00	40.94
ATOM	2278	O	VAL	299	14.321	64.612	23.461	1.00	41.66
ATOM	2279	N	LEU	300	16.337	64.091	24.328	1.00	41.41
ATOM	2280	CA	LEU	300	16.043	64.737	25.600	1.00	42.31
ATOM	2281	CB	LEU	300	16.973	64.224	26.713	1.00	41.48
ATOM	2282	CG	LEU	300	16.943	62.766	27.206	1.00	40.38
ATOM	2283	CD1	LEU	300	17.677	62.711	28.545	1.00	40.14
ATOM	2284	CD2	LEU	300	15.517	62.251	27.380	1.00	38.74
ATOM	2285	C	LEU	300	16.204	66.251	25.444	1.00	43.44
ATOM	2286	O	LEU	300	15.304	67.020	25.806	1.00	43.84
ATOM	2287	N	LEU	301	17.346	66.675	24.898	1.00	43.90
ATOM	2288	CA	LEU	301	17.603	68.100	24.707	1.00	43.85
ATOM	2289	CB	LEU	301	18.895	68.335	23.919	1.00	43.20
ATOM	2290	CG	LEU	301	20.211	67.969	24.613	1.00	43.48
ATOM	2291	CD1	LEU	301	21.385	68.372	23.730	1.00	43.37
ATOM	2292	CD2	LEU	301	20.307	68.675	25.955	1.00	43.71
ATOM	2293	C	LEU	301	16.444	68.738	23.969	1.00	44.11
ATOM	2294	O	LEU	301	16.068	69.875	24.254	1.00	44.38
ATOM	2295	N	ARG	302	15.863	68.007	23.025	1.00	44.45
ATOM	2296	CA	ARG	302	14.753	68.571	22.280	1.00	45.04
ATOM	2297	CB	ARG	302	14.296	67.660	21.148	1.00	45.49
ATOM	2298	CG	ARG	302	13.082	68.256	20.468	1.00	45.91
ATOM	2299	CD	ARG	302	12.391	67.327	19.514	1.00	46.45
ATOM	2300	NE	ARG	302	11.194	67.985	19.007	1.00	47.37
ATOM	2301	CZ	ARG	302	10.423	67.503	18.043	1.00	48.12
ATOM	2302	NH1	ARG	302	10.719	66.344	17.466	1.00	48.80
ATOM	2303	NH2	ARG	302	9.357	68.190	17.657	1.00	47.77
ATOM	2304	C	ARG	302	13.577	68.807	23.196	1.00	45.13
ATOM	2305	O	ARG	302	12.982	69.885	23.198	1.00	45.57
ATOM	2306	N	LEU	303	13.228	67.787	23.966	1.00	45.14
ATOM	2307	CA	LEU	303	12.113	67.918	24.883	1.00	45.18
ATOM	2308	CB	LEU	303	11.952	66.624	25.695	1.00	44.02
ATOM	2309	CG	LEU	303	11.495	65.427	24.846	1.00	42.43
ATOM	2310	CD1	LEU	303	11.365	64.162	25.690	1.00	41.06
ATOM	2311	CD2	LEU	303	10.154	65.784	24.207	1.00	41.96
ATOM	2312	C	LEU	303	12.359	69.133	25.783	1.00	45.83
ATOM	2313	O	LEU	303	11.444	69.919	26.044	1.00	45.85
ATOM	2314	N	VAL	304	13.599	69.302	26.232	1.00	46.44
ATOM	2315	CA	VAL	304	13.943	70.440	27.085	1.00	47.76
ATOM	2316	CB	VAL	304	15.443	70.426	27.496	1.00	47.79
ATOM	2317	CG1	VAL	304	15.866	71.815	27.996	1.00	46.89
ATOM	2318	CG2	VAL	304	15.678	69.386	28.581	1.00	47.81
ATOM	2319	C	VAL	304	13.666	71.764	26.371	1.00	48.44
ATOM	2320	O	VAL	304	12.899	72.596	26.861	1.00	48.95
ATOM	2321	N	ASP	305	14.297	71.946	25.212	1.00	48.52
ATOM	2322	CA	ASP	305	14.143	73.165	24.432	1.00	48.31
ATOM	2323	CB	ASP	305	14.968	73.067	23.143	1.00	49.45
ATOM	2324	CG	ASP	305	16.441	72.715	23.412	1.00	51.00
ATOM	2325	OD1	ASP	305	17.056	73.323	24.317	1.00	50.99
ATOM	2326	OD2	ASP	305	16.994	71.834	22.715	1.00	51.84
ATOM	2327	C	ASP	305	12.677	73.460	24.122	1.00	47.77
ATOM	2328	O	ASP	305	12.341	74.541	23.641	1.00	48.22
ATOM	2329	N	GLU	306	11.799	72.505	24.407	1.00	46.84
ATOM	2330	CA	GLU	306	10.378	72.713	24.176	1.00	46.34
ATOM	2331	CB	GLU	306	9.831	71.683	23.184	1.00	46.20
ATOM	2332	CG	GLU	306	9.866	72.216	21.761	1.00	48.15
ATOM	2333	CD	GLU	306	9.571	71.175	20.692	1.00	49.26

FIG. 400

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ATOM   2334  OE1 GLU   306       8.514  70.499  20.768  1.00 50.03
ATOM   2335  OE2 GLU   306      10.398  71.049  19.759  1.00 49.62
ATOM   2336  C   GLU   306       9.635  72.661  25.493  1.00 45.99
ATOM   2337  O   GLU   306       8.459  72.331  25.550  1.00 45.90
ATOM   2338  N   ASN   307      10.350  72.997  26.560  1.00 46.00
ATOM   2339  CA  ASN   307       9.787  73.029  27.902  1.00 45.60
ATOM   2340  CB  ASN   307       9.033  74.342  28.094  1.00 46.42
ATOM   2341  CG  ASN   307       9.971  75.531  28.224  1.00 46.98
ATOM   2342  OD1 ASN   307      10.435  75.849  29.321  1.00 47.63
ATOM   2343  ND2 ASN   307      10.273  76.181  27.102  1.00 46.93
ATOM   2344  C   ASN   307       8.886  71.853  28.246  1.00 45.05
ATOM   2345  O   ASN   307       7.812  72.029  28.829  1.00 45.19
ATOM   2346  N   LEU   308       9.336  70.650  27.900  1.00 44.24
ATOM   2347  CA  LEU   308       8.575  69.439  28.180  1.00 43.28
ATOM   2348  CB  LEU   308       8.376  68.637  26.893  1.00 43.27
ATOM   2349  CG  LEU   308       7.070  68.825  26.115  1.00 44.09
ATOM   2350  CD1 LEU   308       6.765  70.294  25.935  1.00 44.22
ATOM   2351  CD2 LEU   308       7.182  68.139  24.760  1.00 43.94
ATOM   2352  C   LEU   308       9.287  68.570  29.205  1.00 42.96
ATOM   2353  O   LEU   308       8.688  67.660  29.775  1.00 42.27
ATOM   2354  N   LEU   309      10.560  68.868  29.448  1.00 43.49
ATOM   2355  CA  LEU   309      11.368  68.077  30.371  1.00 44.85
ATOM   2356  CB  LEU   309      12.030  66.936  29.581  1.00 43.53
ATOM   2357  CG  LEU   309      12.958  65.925  30.254  1.00 42.07
ATOM   2358  CD1 LEU   309      12.235  65.226  31.390  1.00 40.83
ATOM   2359  CD2 LEU   309      13.416  64.913  29.212  1.00 42.11
ATOM   2360  C   LEU   309      12.436  68.900  31.108  1.00 46.21
ATOM   2361  O   LEU   309      13.074  69.777  30.518  1.00 46.04
ATOM   2362  N   PHE   310      12.625  68.601  32.397  1.00 47.92
ATOM   2363  CA  PHE   310      13.608  69.293  33.238  1.00 49.25
ATOM   2364  CB  PHE   310      15.013  69.093  32.666  1.00 48.20
ATOM   2365  CG  PHE   310      15.438  67.650  32.590  1.00 47.06
ATOM   2366  CD1 PHE   310      16.338  67.228  31.615  1.00 46.24
ATOM   2367  CD2 PHE   310      14.947  66.715  33.497  1.00 46.63
ATOM   2368  CE1 PHE   310      16.740  65.903  31.540  1.00 45.74
ATOM   2369  CE2 PHE   310      15.344  65.385  33.433  1.00 46.27
ATOM   2370  CZ  PHE   310      16.243  64.978  32.451  1.00 45.93
ATOM   2371  C   PHE   310      13.292  70.785  33.345  1.00 51.16
ATOM   2372  O   PHE   310      14.185  71.616  33.561  1.00 50.84
ATOM   2373  N   HIS   311      12.009  71.109  33.183  1.00 53.40
ATOM   2374  CA  HIS   311      11.529  72.482  33.262  1.00 55.80
ATOM   2375  CB  HIS   311      11.744  73.012  34.683  1.00 57.57
ATOM   2376  CG  HIS   311      11.212  72.098  35.745  1.00 59.78
ATOM   2377  CD2 HIS   311      11.848  71.363  36.689  1.00 60.29
ATOM   2378  ND1 HIS   311       9.867  71.815  35.879  1.00 60.36
ATOM   2379  CE1 HIS   311       9.699  70.944  36.860  1.00 60.99
ATOM   2380  NE2 HIS   311      10.885  70.654  37.368  1.00 60.85
ATOM   2381  C   HIS   311      12.214  73.384  32.236  1.00 56.24
ATOM   2382  O   HIS   311      12.288  74.608  32.415  1.00 56.87
ATOM   2383  N   GLY   312      12.705  72.772  31.159  1.00 55.96
ATOM   2384  CA  GLY   312      13.366  73.522  30.109  1.00 55.87
ATOM   2385  C   GLY   312      14.820  73.804  30.420  1.00 56.16
ATOM   2386  O   GLY   312      15.563  74.264  29.562  1.00 56.58
ATOM   2387  N   GLU   313      15.235  73.519  31.646  1.00 56.52
ATOM   2388  CA  GLU   313      16.612  73.765  32.048  1.00 57.69
ATOM   2389  CB  GLU   313      16.621  74.379  33.447  1.00 59.84
ATOM   2390  CG  GLU   313      15.849  75.698  33.515  1.00 63.16
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FIG. 4PP

```
ATOM   2391  CD  GLU  313      15.388  76.061  34.925  1.00 65.16
ATOM   2392  OE1 GLU  313      14.554  75.315  35.503  1.00 66.01
ATOM   2393  OE2 GLU  313      15.858  77.096  35.455  1.00 66.34
ATOM   2394  C   GLU  313      17.439  72.484  32.011  1.00 57.06
ATOM   2395  O   GLU  313      17.155  71.529  32.728  1.00 57.01
ATOM   2396  N   ALA  314      18.463  72.472  31.169  1.00 56.56
ATOM   2397  CA  ALA  314      19.316  71.305  31.029  1.00 56.76
ATOM   2398  CB  ALA  314      19.454  70.939  29.557  1.00 56.47
ATOM   2399  C   ALA  314      20.699  71.490  31.643  1.00 56.94
ATOM   2400  O   ALA  314      21.310  72.558  31.527  1.00 57.46
ATOM   2401  N   SER  315      21.183  70.422  32.276  1.00 56.73
ATOM   2402  CA  SER  315      22.487  70.383  32.932  1.00 56.15
ATOM   2403  CB  SER  315      22.666  69.029  33.624  1.00 56.44
ATOM   2404  OG  SER  315      23.981  68.868  34.130  1.00 57.39
ATOM   2405  C   SER  315      23.673  70.627  32.003  1.00 56.00
ATOM   2406  O   SER  315      23.595  70.416  30.793  1.00 55.42
ATOM   2407  N   GLU  316      24.776  71.070  32.598  1.00 56.67
ATOM   2408  CA  GLU  316      26.012  71.346  31.875  1.00 57.46
ATOM   2409  CB  GLU  316      27.111  71.754  32.860  1.00 58.71
ATOM   2410  CG  GLU  316      28.458  72.050  32.206  1.00 60.34
ATOM   2411  CD  GLU  316      28.442  73.343  31.406  1.00 61.64
ATOM   2412  OE1 GLU  316      28.288  74.420  32.031  1.00 62.41
ATOM   2413  OE2 GLU  316      28.574  73.280  30.160  1.00 61.76
ATOM   2414  C   GLU  316      26.442  70.078  31.161  1.00 57.35
ATOM   2415  O   GLU  316      26.770  70.088  29.972  1.00 57.68
ATOM   2416  N   GLN  317      26.439  68.988  31.920  1.00 56.84
ATOM   2417  CA  GLN  317      26.817  67.677  31.427  1.00 56.23
ATOM   2418  CB  GLN  317      26.760  66.669  32.580  1.00 55.93
ATOM   2419  CG  GLN  317      27.504  67.113  33.840  1.00 55.46
ATOM   2420  CD  GLN  317      27.063  66.355  35.085  1.00 55.01
ATOM   2421  OE1 GLN  317      27.246  65.140  35.194  1.00 54.83
ATOM   2422  NE2 GLN  317      26.468  67.074  36.029  1.00 54.68
ATOM   2423  C   GLN  317      25.902  67.210  30.290  1.00 56.37
ATOM   2424  O   GLN  317      26.376  66.634  29.312  1.00 56.16
ATOM   2425  N   LEU  318      24.599  67.476  30.412  1.00 56.41
ATOM   2426  CA  LEU  318      23.616  67.043  29.413  1.00 56.48
ATOM   2427  CB  LEU  318      22.190  67.333  29.890  1.00 55.59
ATOM   2428  CG  LEU  318      21.084  66.700  29.034  1.00 54.71
ATOM   2429  CD1 LEU  318      21.090  65.191  29.231  1.00 53.88
ATOM   2430  CD2 LEU  318      19.731  67.268  29.422  1.00 54.28
ATOM   2431  C   LEU  318      23.784  67.621  28.017  1.00 56.99
ATOM   2432  O   LEU  318      23.692  66.893  27.029  1.00 57.21
ATOM   2433  N   ARG  319      24.011  68.924  27.919  1.00 57.16
ATOM   2434  CA  ARG  319      24.177  69.530  26.606  1.00 57.68
ATOM   2435  CB  ARG  319      23.870  71.026  26.690  1.00 59.32
ATOM   2436  CG  ARG  319      22.420  71.284  27.105  1.00 62.20
ATOM   2437  CD  ARG  319      22.125  72.743  27.401  1.00 64.53
ATOM   2438  NE  ARG  319      20.758  72.927  27.892  1.00 66.89
ATOM   2439  CZ  ARG  319      20.297  74.055  28.433  1.00 68.29
ATOM   2440  NH1 ARG  319      21.096  75.112  28.555  1.00 68.30
ATOM   2441  NH2 ARG  319      19.034  74.127  28.851  1.00 68.25
ATOM   2442  C   ARG  319      25.587  69.278  26.081  1.00 57.09
ATOM   2443  O   ARG  319      26.049  69.951  25.160  1.00 57.05
ATOM   2444  N   THR  320      26.246  68.277  26.667  1.00 56.25
ATOM   2445  CA  THR  320      27.612  67.888  26.318  1.00 55.15
ATOM   2446  CB  THR  320      28.478  67.836  27.589  1.00 54.85
ATOM   2447  OG1 THR  320      28.601  69.158  28.133  1.00 54.94
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FIG. 4QQ

```
ATOM   2448  CG2 THR   320      29.854  67.262  27.287  1.00 54.63
ATOM   2449  C   THR   320      27.689  66.524  25.613  1.00 55.04
ATOM   2450  O   THR   320      27.476  65.480  26.229  1.00 55.13
ATOM   2451  N   ARG   321      28.017  66.536  24.326  1.00 54.38
ATOM   2452  CA  ARG   321      28.106  65.304  23.545  1.00 54.36
ATOM   2453  CB  ARG   321      28.841  65.586  22.236  1.00 56.05
ATOM   2454  CG  ARG   321      28.153  66.651  21.402  1.00 59.03
ATOM   2455  CD  ARG   321      28.943  67.013  20.156  1.00 61.60
ATOM   2456  NE  ARG   321      28.331  68.123  19.426  1.00 63.68
ATOM   2457  CZ  ARG   321      28.909  68.753  18.406  1.00 65.43
ATOM   2458  NH1 ARG   321      30.119  68.381  17.997  1.00 65.83
ATOM   2459  NH2 ARG   321      28.280  69.750  17.792  1.00 65.76
ATOM   2460  C   ARG   321      28.765  64.123  24.262  1.00 52.97
ATOM   2461  O   ARG   321      29.885  64.234  24.758  1.00 53.13
ATOM   2462  N   GLY   322      28.056  62.996  24.316  1.00 51.39
ATOM   2463  CA  GLY   322      28.592  61.802  24.950  1.00 49.22
ATOM   2464  C   GLY   322      28.198  61.609  26.402  1.00 48.17
ATOM   2465  O   GLY   322      28.450  60.550  26.986  1.00 48.17
ATOM   2466  N   ALA   323      27.574  62.627  26.988  1.00 46.66
ATOM   2467  CA  ALA   323      27.150  62.573  28.385  1.00 44.99
ATOM   2468  CB  ALA   323      26.462  63.861  28.761  1.00 45.87
ATOM   2469  C   ALA   323      26.224  61.403  28.676  1.00 43.43
ATOM   2470  O   ALA   323      26.514  60.562  29.530  1.00 43.02
ATOM   2471  N   PHE   324      25.094  61.361  27.981  1.00 41.61
ATOM   2472  CA  PHE   324      24.147  60.282  28.185  1.00 40.44
ATOM   2473  CB  PHE   324      22.797  60.631  27.564  1.00 38.94
ATOM   2474  CG  PHE   324      21.644  59.988  28.262  1.00 38.08
ATOM   2475  CD1 PHE   324      21.047  60.613  29.360  1.00 37.48
ATOM   2476  CD2 PHE   324      21.185  58.733  27.860  1.00 36.96
ATOM   2477  CE1 PHE   324      20.010  59.998  30.050  1.00 37.11
ATOM   2478  CE2 PHE   324      20.146  58.105  28.542  1.00 37.79
ATOM   2479  CZ  PHE   324      19.555  58.739  29.643  1.00 37.73
ATOM   2480  C   PHE   324      24.721  59.033  27.525  1.00 40.11
ATOM   2481  O   PHE   324      24.785  58.937  26.289  1.00 40.76
ATOM   2482  N   GLU   325      25.129  58.072  28.350  1.00 39.06
ATOM   2483  CA  GLU   325      25.740  56.851  27.844  1.00 37.85
ATOM   2484  CB  GLU   325      26.846  56.418  28.781  1.00 38.17
ATOM   2485  CG  GLU   325      27.790  57.528  29.085  1.00 40.68
ATOM   2486  CD  GLU   325      28.922  57.075  29.951  1.00 42.47
ATOM   2487  OE1 GLU   325      28.653  56.608  31.086  1.00 44.06
ATOM   2488  OE2 GLU   325      30.080  57.181  29.490  1.00 44.51
ATOM   2489  C   GLU   325      24.799  55.693  27.641  1.00 36.60
ATOM   2490  O   GLU   325      23.903  55.445  28.447  1.00 37.31
ATOM   2491  N   THR   326      25.019  54.968  26.554  1.00 35.30
ATOM   2492  CA  THR   326      24.193  53.816  26.245  1.00 33.37
ATOM   2493  CB  THR   326      24.875  52.921  25.207  1.00 31.58
ATOM   2494  OG1 THR   326      24.934  53.617  23.956  1.00 29.82
ATOM   2495  CG2 THR   326      24.113  51.619  25.041  1.00 29.94
ATOM   2496  C   THR   326      23.951  53.016  27.515  1.00 33.05
ATOM   2497  O   THR   326      22.846  52.528  27.742  1.00 33.99
ATOM   2498  N   ARG   327      24.981  52.902  28.349  1.00 32.29
ATOM   2499  CA  ARG   327      24.859  52.148  29.588  1.00 31.76
ATOM   2500  CB  ARG   327      26.146  52.245  30.417  1.00 33.30
ATOM   2501  CG  ARG   327      26.226  51.162  31.485  1.00 36.71
ATOM   2502  CD  ARG   327      27.596  51.043  32.177  1.00 38.88
ATOM   2503  NE  ARG   327      27.795  52.024  33.249  1.00 40.62
ATOM   2504  CZ  ARG   327      28.274  53.255  33.069  1.00 41.13
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FIG. 4RR

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ATOM   2505  NH1 ARG   327      28.615  53.670  31.846  1.00 40.49
ATOM   2506  NH2 ARG   327      28.393  54.078  34.113  1.00 40.82
ATOM   2507  C   ARG   327      23.681  52.691  30.387  1.00 30.62
ATOM   2508  O   ARG   327      22.888  51.930  30.940  1.00 29.96
ATOM   2509  N   PHE   328      23.559  54.014  30.425  1.00 29.60
ATOM   2510  CA  PHE   328      22.479  54.660  31.154  1.00 28.70
ATOM   2511  CB  PHE   328      22.632  56.176  31.069  1.00 28.03
ATOM   2512  CG  PHE   328      23.903  56.684  31.686  1.00 27.73
ATOM   2513  CD1 PHE   328      24.337  57.975  31.439  1.00 27.37
ATOM   2514  CD2 PHE   328      24.678  55.857  32.505  1.00 28.92
ATOM   2515  CE1 PHE   328      25.526  58.437  31.992  1.00 28.75
ATOM   2516  CE2 PHE   328      25.871  56.305  33.069  1.00 28.74
ATOM   2517  CZ  PHE   328      26.298  57.599  32.812  1.00 28.68
ATOM   2518  C   PHE   328      21.135  54.226  30.590  1.00 29.06
ATOM   2519  O   PHE   328      20.189  53.953  31.351  1.00 29.59
ATOM   2520  N   VAL   329      21.057  54.154  29.257  1.00 28.40
ATOM   2521  CA  VAL   329      19.830  53.735  28.587  1.00 26.44
ATOM   2522  CB  VAL   329      20.040  53.552  27.059  1.00 25.14
ATOM   2523  CG1 VAL   329      18.737  53.107  26.387  1.00 22.55
ATOM   2524  CG2 VAL   329      20.542  54.841  26.444  1.00 23.05
ATOM   2525  C   VAL   329      19.388  52.399  29.166  1.00 27.98
ATOM   2526  O   VAL   329      18.240  52.239  29.576  1.00 27.88
ATOM   2527  N   SER   330      20.308  51.442  29.219  1.00 28.76
ATOM   2528  CA  SER   330      19.966  50.117  29.718  1.00 30.08
ATOM   2529  CB  SER   330      21.136  49.171  29.534  1.00 30.45
ATOM   2530  OG  SER   330      20.720  47.852  29.822  1.00 31.92
ATOM   2531  C   SER   330      19.534  50.107  31.172  1.00 31.40
ATOM   2532  O   SER   330      18.690  49.298  31.577  1.00 31.74
ATOM   2533  N   GLN   331      20.118  50.993  31.972  1.00 32.45
ATOM   2534  CA  GLN   331      19.745  51.061  33.381  1.00 33.16
ATOM   2535  CB  GLN   331      20.668  51.992  34.151  1.00 33.58
ATOM   2536  CG  GLN   331      22.093  51.540  34.194  1.00 35.83
ATOM   2537  CD  GLN   331      22.947  52.534  34.919  1.00 37.72
ATOM   2538  OE1 GLN   331      22.626  52.927  36.043  1.00 39.62
ATOM   2539  NE2 GLN   331      24.042  52.958  34.291  1.00 38.98
ATOM   2540  C   GLN   331      18.327  51.591  33.482  1.00 33.78
ATOM   2541  O   GLN   331      17.428  50.881  33.938  1.00 34.06
ATOM   2542  N   VAL   332      18.129  52.835  33.038  1.00 33.77
ATOM   2543  CA  VAL   332      16.808  53.457  33.097  1.00 33.65
ATOM   2544  CB  VAL   332      16.760  54.791  32.282  1.00 32.19
ATOM   2545  CG1 VAL   332      17.279  54.584  30.905  1.00 33.04
ATOM   2546  CG2 VAL   332      15.340  55.312  32.215  1.00 31.67
ATOM   2547  C   VAL   332      15.695  52.505  32.638  1.00 34.20
ATOM   2548  O   VAL   332      14.571  52.566  33.139  1.00 34.51
ATOM   2549  N   GLU   333      16.001  51.607  31.711  1.00 34.30
ATOM   2550  CA  GLU   333      14.981  50.676  31.258  1.00 34.92
ATOM   2551  CB  GLU   333      15.210  50.289  29.795  1.00 34.40
ATOM   2552  CG  GLU   333      14.893  51.413  28.837  1.00 33.07
ATOM   2553  CD  GLU   333      14.806  50.956  27.409  1.00 31.80
ATOM   2554  OE1 GLU   333      13.983  50.060  27.114  1.00 31.65
ATOM   2555  OE2 GLU   333      15.561  51.504  26.581  1.00 31.72
ATOM   2556  C   GLU   333      14.949  49.438  32.135  1.00 35.76
ATOM   2557  O   GLU   333      14.163  48.520  31.911  1.00 35.73
ATOM   2558  N   SER   334      15.814  49.419  33.138  1.00 36.91
ATOM   2559  CA  SER   334      15.876  48.307  34.071  1.00 38.13
ATOM   2560  CB  SER   334      17.328  47.934  34.346  1.00 39.38
ATOM   2561  OG  SER   334      17.460  46.524  34.468  1.00 41.52
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FIG. 4SS

ATOM	2562	C	SER	334	15.201	48.747	35.362	1.00	37.93
ATOM	2563	O	SER	334	15.053	47.973	36.306	1.00	38.63
ATOM	2564	N	ASP	335	14.807	50.014	35.385	1.00	38.51
ATOM	2565	CA	ASP	335	14.133	50.619	36.521	1.00	38.59
ATOM	2566	CB	ASP	335	13.776	52.061	36.173	1.00	39.10
ATOM	2567	CG	ASP	335	13.346	52.864	37.373	1.00	39.89
ATOM	2568	OD1	ASP	335	12.278	52.547	37.950	1.00	40.30
ATOM	2569	OD2	ASP	335	14.079	53.816	37.737	1.00	39.90
ATOM	2570	C	ASP	335	12.876	49.809	36.840	1.00	39.11
ATOM	2571	O	ASP	335	12.241	49.249	35.945	1.00	39.03
ATOM	2572	N	THR	336	12.517	49.768	38.119	1.00	39.68
ATOM	2573	CA	THR	336	11.372	48.999	38.605	1.00	39.94
ATOM	2574	CB	THR	336	11.773	48.297	39.896	1.00	39.68
ATOM	2575	OG1	THR	336	12.901	47.464	39.630	1.00	40.95
ATOM	2576	CG2	THR	336	10.650	47.452	40.426	1.00	39.84
ATOM	2577	C	THR	336	10.043	49.735	38.853	1.00	40.52
ATOM	2578	O	THR	336	8.984	49.108	38.931	1.00	40.91
ATOM	2579	N	GLY	337	10.085	51.054	38.970	1.00	40.80
ATOM	2580	CA	GLY	337	8.870	51.804	39.234	1.00	41.83
ATOM	2581	C	GLY	337	9.307	52.948	40.112	1.00	42.60
ATOM	2582	O	GLY	337	8.990	54.105	39.865	1.00	43.33
ATOM	2583	N	ASP	338	10.043	52.604	41.156	1.00	43.47
ATOM	2584	CA	ASP	338	10.606	53.589	42.059	1.00	44.40
ATOM	2585	CB	ASP	338	11.354	52.868	43.175	1.00	44.83
ATOM	2586	CG	ASP	338	12.303	51.808	42.637	1.00	45.34
ATOM	2587	OD1	ASP	338	11.879	51.032	41.751	1.00	46.12
ATOM	2588	OD2	ASP	338	13.465	51.742	43.087	1.00	45.59
ATOM	2589	C	ASP	338	11.597	54.296	41.142	1.00	44.84
ATOM	2590	O	ASP	338	12.605	53.709	40.756	1.00	45.53
ATOM	2591	N	ARG	339	11.310	55.533	40.763	1.00	44.81
ATOM	2592	CA	ARG	339	12.208	56.256	39.874	1.00	45.11
ATOM	2593	CB	ARG	339	11.702	57.687	39.654	1.00	45.72
ATOM	2594	CG	ARG	339	10.466	57.799	38.783	1.00	46.11
ATOM	2595	CD	ARG	339	9.201	57.413	39.521	1.00	46.99
ATOM	2596	NE	ARG	339	8.041	57.492	38.633	1.00	47.58
ATOM	2597	CZ	ARG	339	6.780	57.326	39.017	1.00	47.30
ATOM	2598	NH1	ARG	339	6.492	57.068	40.287	1.00	47.38
ATOM	2599	NH2	ARG	339	5.806	57.413	38.123	1.00	47.44
ATOM	2600	C	ARG	339	13.637	56.295	40.419	1.00	44.98
ATOM	2601	O	ARG	339	14.466	57.084	39.960	1.00	44.83
ATOM	2602	N	LYS	340	13.922	55.441	41.394	1.00	44.75
ATOM	2603	CA	LYS	340	15.238	55.394	42.001	1.00	45.05
ATOM	2604	CB	LYS	340	15.341	54.179	42.917	1.00	46.19
ATOM	2605	CG	LYS	340	14.358	54.250	44.081	1.00	47.87
ATOM	2606	CD	LYS	340	14.598	53.154	45.094	1.00	49.25
ATOM	2607	CE	LYS	340	13.365	52.949	45.957	1.00	50.44
ATOM	2608	NZ	LYS	340	13.353	51.589	46.598	1.00	51.78
ATOM	2609	C	LYS	340	16.398	55.422	41.014	1.00	44.66
ATOM	2610	O	LYS	340	17.186	56.372	41.026	1.00	44.90
ATOM	2611	N	GLN	341	16.509	54.408	40.155	1.00	43.94
ATOM	2612	CA	GLN	341	17.603	54.362	39.174	1.00	42.93
ATOM	2613	CB	GLN	341	17.598	53.028	38.435	1.00	45.04
ATOM	2614	CG	GLN	341	18.035	51.860	39.289	1.00	48.03
ATOM	2615	CD	GLN	341	18.758	50.801	38.482	1.00	49.69
ATOM	2616	OE1	GLN	341	19.731	51.101	37.779	1.00	50.67
ATOM	2617	NE2	GLN	341	18.297	49.556	38.581	1.00	50.43
ATOM	2618	C	GLN	341	17.616	55.497	38.146	1.00	40.93

FIG. 4TT

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ATOM   2619  O   GLN   341      18.672  56.057  37.839  1.00 38.85
ATOM   2620  N   ILE   342      16.449  55.824  37.600  1.00 39.61
ATOM   2621  CA  ILE   342      16.364  56.905  36.624  1.00 39.07
ATOM   2622  CB  ILE   342      14.920  57.110  36.130  1.00 39.24
ATOM   2623  CG2 ILE   342      14.880  58.226  35.107  1.00 39.19
ATOM   2624  CG1 ILE   342      14.392  55.817  35.501  1.00 39.87
ATOM   2625  CD1 ILE   342      12.945  55.902  35.070  1.00 40.76
ATOM   2626  C   ILE   342      16.832  58.185  37.301  1.00 38.43
ATOM   2627  O   ILE   342      17.704  58.892  36.795  1.00 37.48
ATOM   2628  N   TYR   343      16.240  58.466  38.456  1.00 38.93
ATOM   2629  CA  TYR   343      16.580  59.647  39.236  1.00 39.71
ATOM   2630  CB  TYR   343      15.813  59.656  40.567  1.00 40.97
ATOM   2631  CG  TYR   343      16.173  60.835  41.448  1.00 42.53
ATOM   2632  CD1 TYR   343      15.344  61.954  41.521  1.00 43.30
ATOM   2633  CE1 TYR   343      15.730  63.092  42.228  1.00 44.58
ATOM   2634  CD2 TYR   343      17.397  60.880  42.119  1.00 43.04
ATOM   2635  CE2 TYR   343      17.791  62.014  42.826  1.00 43.55
ATOM   2636  CZ  TYR   343      16.958  63.117  42.872  1.00 44.31
ATOM   2637  OH  TYR   343      17.369  64.260  43.523  1.00 45.74
ATOM   2638  C   TYR   343      18.070  59.635  39.532  1.00 39.93
ATOM   2639  O   TYR   343      18.789  60.598  39.262  1.00 40.28
ATOM   2640  N   ASN   344      18.525  58.529  40.098  1.00 40.14
ATOM   2641  CA  ASN   344      19.924  58.371  40.460  1.00 40.97
ATOM   2642  CB  ASN   344      20.146  56.958  40.989  1.00 42.94
ATOM   2643  CG  ASN   344      21.287  56.880  41.977  1.00 44.68
ATOM   2644  OD1 ASN   344      22.448  57.137  41.628  1.00 46.05
ATOM   2645  ND2 ASN   344      20.965  56.531  43.225  1.00 44.93
ATOM   2646  C   ASN   344      20.869  58.649  39.292  1.00 40.46
ATOM   2647  O   ASN   344      21.946  59.208  39.483  1.00 40.33
ATOM   2648  N   ILE   345      20.460  58.262  38.085  1.00 40.50
ATOM   2649  CA  ILE   345      21.280  58.467  36.890  1.00 39.89
ATOM   2650  CB  ILE   345      20.803  57.555  35.720  1.00 39.76
ATOM   2651  CG2 ILE   345      21.597  57.849  34.448  1.00 38.62
ATOM   2652  CG1 ILE   345      20.966  56.090  36.114  1.00 38.74
ATOM   2653  CD1 ILE   345      20.201  55.151  35.242  1.00 38.61
ATOM   2654  C   ILE   345      21.247  59.924  36.434  1.00 39.80
ATOM   2655  O   ILE   345      22.281  60.490  36.074  1.00 39.67
ATOM   2656  N   LEU   346      20.062  60.529  36.449  1.00 39.59
ATOM   2657  CA  LEU   346      19.912  61.923  36.029  1.00 39.58
ATOM   2658  CB  LEU   346      18.434  62.255  35.818  1.00 37.79
ATOM   2659  CG  LEU   346      17.809  61.528  34.625  1.00 36.58
ATOM   2660  CD1 LEU   346      16.277  61.599  34.684  1.00 35.18
ATOM   2661  CD2 LEU   346      18.363  62.145  33.337  1.00 35.05
ATOM   2662  C   LEU   346      20.519  62.892  37.034  1.00 40.82
ATOM   2663  O   LEU   346      21.177  63.857  36.654  1.00 41.02
ATOM   2664  N   SER   347      20.298  62.646  38.322  1.00 42.34
ATOM   2665  CA  SER   347      20.859  63.530  39.339  1.00 43.44
ATOM   2666  CB  SER   347      20.491  63.042  40.745  1.00 43.90
ATOM   2667  OG  SER   347      20.665  61.639  40.868  1.00 45.32
ATOM   2668  C   SER   347      22.368  63.556  39.156  1.00 43.44
ATOM   2669  O   SER   347      22.974  64.624  39.051  1.00 44.11
ATOM   2670  N   THR   348      22.969  62.374  39.096  1.00 43.10
ATOM   2671  CA  THR   348      24.407  62.285  38.909  1.00 42.97
ATOM   2672  CB  THR   348      24.853  60.830  38.700  1.00 42.31
ATOM   2673  OG1 THR   348      24.666  60.096  39.918  1.00 42.08
ATOM   2674  CG2 THR   348      26.322  60.780  38.282  1.00 40.85
ATOM   2675  C   THR   348      24.798  63.093  37.683  1.00 43.25
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FIG. 4UU

ATOM	2676	O	THR	348	25.796	63.813	37.680	1.00	43.52
ATOM	2677	N	LEU	349	23.990	62.982	36.640	1.00	43.57
ATOM	2678	CA	LEU	349	24.271	63.697	35.412	1.00	44.17
ATOM	2679	CB	LEU	349	23.343	63.180	34.311	1.00	44.43
ATOM	2680	CG	LEU	349	23.787	63.204	32.847	1.00	44.86
ATOM	2681	CD1	LEU	349	25.198	62.658	32.688	1.00	44.59
ATOM	2682	CD2	LEU	349	22.790	62.375	32.046	1.00	44.64
ATOM	2683	C	LEU	349	24.102	65.201	35.638	1.00	44.32
ATOM	2684	O	LEU	349	24.317	66.003	34.726	1.00	45.33
ATOM	2685	N	GLY	350	23.722	65.574	36.862	1.00	43.94
ATOM	2686	CA	GLY	350	23.559	66.981	37.210	1.00	43.15
ATOM	2687	C	GLY	350	22.167	67.570	37.038	1.00	42.49
ATOM	2688	O	GLY	350	22.024	68.752	36.703	1.00	41.70
ATOM	2689	N	LEU	351	21.143	66.758	37.288	1.00	41.97
ATOM	2690	CA	LEU	351	19.758	67.197	37.132	1.00	41.45
ATOM	2691	CB	LEU	351	19.194	66.676	35.812	1.00	40.99
ATOM	2692	CG	LEU	351	19.875	67.115	34.522	1.00	40.66
ATOM	2693	CD1	LEU	351	19.516	66.144	33.416	1.00	41.63
ATOM	2694	CD2	LEU	351	19.453	68.533	34.172	1.00	40.77
ATOM	2695	C	LEU	351	18.858	66.718	38.262	1.00	41.15
ATOM	2696	O	LEU	351	19.170	65.760	38.973	1.00	40.88
ATOM	2697	N	ARG	352	17.720	67.379	38.410	1.00	41.10
ATOM	2698	CA	ARG	352	16.782	67.007	39.457	1.00	41.25
ATOM	2699	CB	ARG	352	16.614	68.173	40.431	1.00	42.65
ATOM	2700	CG	ARG	352	17.929	68.581	41.070	1.00	43.68
ATOM	2701	CD	ARG	352	18.504	67.421	41.851	1.00	45.59
ATOM	2702	NE	ARG	352	19.960	67.478	41.917	1.00	47.73
ATOM	2703	CZ	ARG	352	20.715	66.567	42.521	1.00	48.77
ATOM	2704	NH1	ARG	352	20.143	65.524	43.119	1.00	49.05
ATOM	2705	NH2	ARG	352	22.038	66.700	42.519	1.00	49.14
ATOM	2706	C	ARG	352	15.458	66.621	38.827	1.00	39.59
ATOM	2707	O	ARG	352	14.512	67.399	38.793	1.00	40.34
ATOM	2708	N	PRO	353	15.378	65.388	38.324	1.00	38.06
ATOM	2709	CD	PRO	353	16.325	64.285	38.555	1.00	37.28
ATOM	2710	CA	PRO	353	14.159	64.901	37.683	1.00	37.45
ATOM	2711	CB	PRO	353	14.595	63.552	37.134	1.00	37.27
ATOM	2712	CG	PRO	353	15.491	63.064	38.232	1.00	36.92
ATOM	2713	C	PRO	353	12.998	64.763	38.650	1.00	36.35
ATOM	2714	O	PRO	353	13.180	64.360	39.791	1.00	36.28
ATOM	2715	N	SER	354	11.805	65.110	38.194	1.00	35.82
ATOM	2716	CA	SER	354	10.625	64.951	39.028	1.00	36.40
ATOM	2717	CB	SER	354	9.570	66.010	38.698	1.00	35.94
ATOM	2718	OG	SER	354	8.944	65.725	37.459	1.00	35.63
ATOM	2719	C	SER	354	10.091	63.570	38.653	1.00	36.41
ATOM	2720	O	SER	354	10.592	62.948	37.716	1.00	37.42
ATOM	2721	N	THR	355	9.087	63.091	39.375	1.00	36.02
ATOM	2722	CA	THR	355	8.493	61.790	39.099	1.00	35.68
ATOM	2723	CB	THR	355	7.200	61.615	39.923	1.00	36.38
ATOM	2724	OG1	THR	355	7.525	61.645	41.316	1.00	37.75
ATOM	2725	CG2	THR	355	6.510	60.293	39.598	1.00	36.44
ATOM	2726	C	THR	355	8.161	61.633	37.609	1.00	35.80
ATOM	2727	O	THR	355	8.319	60.548	37.029	1.00	34.73
ATOM	2728	N	THR	356	7.698	62.720	36.994	1.00	35.28
ATOM	2729	CA	THR	356	7.336	62.690	35.586	1.00	35.39
ATOM	2730	CB	THR	356	6.287	63.774	35.263	1.00	35.59
ATOM	2731	OG1	THR	356	6.651	64.990	35.925	1.00	35.39
ATOM	2732	CG2	THR	356	4.892	63.331	35.719	1.00	34.33

FIG. 4VV

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ATOM   2733  C   THR  356      8.542  62.848  34.662  1.00 35.30
ATOM   2734  O   THR  356      8.560  62.285  33.559  1.00 34.91
ATOM   2735  N   ASP  357      9.537  63.624  35.089  1.00 35.07
ATOM   2736  CA  ASP  357     10.740  63.782  34.277  1.00 35.80
ATOM   2737  CB  ASP  357     11.804  64.598  35.012  1.00 36.76
ATOM   2738  CG  ASP  357     11.451  66.077  35.116  1.00 38.19
ATOM   2739  OD1 ASP  357     11.475  66.778  34.071  1.00 37.60
ATOM   2740  OD2 ASP  357     11.158  66.538  36.249  1.00 38.76
ATOM   2741  C   ASP  357     11.277  62.373  34.039  1.00 35.97
ATOM   2742  O   ASP  357     11.460  61.942  32.901  1.00 36.94
ATOM   2743  N   CYS  358     11.498  61.649  35.131  1.00 35.67
ATOM   2744  CA  CYS  358     12.013  60.293  35.057  1.00 35.44
ATOM   2745  CB  CYS  358     12.051  59.658  36.447  1.00 35.93
ATOM   2746  SG  CYS  358     13.247  60.410  37.575  1.00 35.81
ATOM   2747  C   CYS  358     11.177  59.433  34.138  1.00 34.88
ATOM   2748  O   CYS  358     11.711  58.698  33.308  1.00 35.87
ATOM   2749  N   ASP  359      9.863  59.517  34.290  1.00 34.10
ATOM   2750  CA  ASP  359      8.960  58.729  33.464  1.00 33.10
ATOM   2751  CB  ASP  359      7.519  58.964  33.910  1.00 35.03
ATOM   2752  CG  ASP  359      7.118  58.058  35.062  1.00 36.65
ATOM   2753  OD1 ASP  359      7.950  57.850  35.975  1.00 38.15
ATOM   2754  OD2 ASP  359      5.969  57.561  35.055  1.00 37.12
ATOM   2755  C   ASP  359      9.130  59.058  31.985  1.00 31.16
ATOM   2756  O   ASP  359      9.090  58.170  31.133  1.00 30.01
ATOM   2757  N   ILE  360      9.325  60.334  31.682  1.00 29.54
ATOM   2758  CA  ILE  360      9.524  60.741  30.300  1.00 28.61
ATOM   2759  CB  ILE  360      9.546  62.273  30.162  1.00 27.75
ATOM   2760  CG2 ILE  360     10.255  62.668  28.874  1.00 27.01
ATOM   2761  CG1 ILE  360      8.112  62.818  30.235  1.00 26.18
ATOM   2762  CD1 ILE  360      8.024  64.322  30.190  1.00 23.23
ATOM   2763  C   ILE  360     10.857  60.176  29.825  1.00 29.21
ATOM   2764  O   ILE  360     10.919  59.480  28.805  1.00 29.88
ATOM   2765  N   VAL  361     11.923  60.466  30.569  1.00 28.39
ATOM   2766  CA  VAL  361     13.248  59.971  30.219  1.00 28.01
ATOM   2767  CB  VAL  361     14.258  60.256  31.342  1.00 27.73
ATOM   2768  CG1 VAL  361     15.575  59.551  31.055  1.00 27.43
ATOM   2769  CG2 VAL  361     14.492  61.759  31.453  1.00 27.76
ATOM   2770  C   VAL  361     13.245  58.464  29.919  1.00 27.74
ATOM   2771  O   VAL  361     14.055  57.982  29.107  1.00 27.40
ATOM   2772  N   ARG  362     12.341  57.719  30.556  1.00 27.72
ATOM   2773  CA  ARG  362     12.277  56.275  30.325  1.00 27.95
ATOM   2774  CB  ARG  362     11.523  55.571  31.455  1.00 29.48
ATOM   2775  CG  ARG  362     11.137  54.147  31.101  1.00 31.97
ATOM   2776  CD  ARG  362     10.900  53.266  32.308  1.00 33.93
ATOM   2777  NE  ARG  362     10.930  51.859  31.893  1.00 37.37
ATOM   2778  CZ  ARG  362     10.938  50.817  32.725  1.00 37.52
ATOM   2779  NH1 ARG  362     10.920  51.010  34.043  1.00 38.72
ATOM   2780  NH2 ARG  362     10.960  49.582  32.230  1.00 36.06
ATOM   2781  C   ARG  362     11.614  55.959  28.994  1.00 27.88
ATOM   2782  O   ARG  362     12.016  55.032  28.289  1.00 29.02
ATOM   2783  N   ARG  363     10.586  56.728  28.660  1.00 27.31
ATOM   2784  CA  ARG  363      9.866  56.564  27.400  1.00 25.77
ATOM   2785  CB  ARG  363      8.641  57.486  27.374  1.00 26.51
ATOM   2786  CG  ARG  363      7.530  57.084  28.318  1.00 26.30
ATOM   2787  CD  ARG  363      6.730  55.929  27.739  1.00 28.36
ATOM   2788  NE  ARG  363      6.259  56.216  26.380  1.00 30.91
ATOM   2789  CZ  ARG  363      6.872  55.826  25.260  1.00 31.55
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FIG. 4WW

ATOM	2790	NH1	ARG	363	7.992	55.112	25.315	1.00	33.18
ATOM	2791	NH2	ARG	363	6.370	56.158	24.077	1.00	32.30
ATOM	2792	C	ARG	363	10.817	56.949	26.272	1.00	24.71
ATOM	2793	O	ARG	363	10.748	56.392	25.175	1.00	24.40
ATOM	2794	N	ALA	364	11.706	57.905	26.540	1.00	23.90
ATOM	2795	CA	ALA	364	12.653	58.339	25.507	1.00	24.48
ATOM	2796	CB	ALA	364	13.463	59.545	25.969	1.00	23.15
ATOM	2797	C	ALA	364	13.571	57.176	25.226	1.00	25.01
ATOM	2798	O	ALA	364	13.854	56.872	24.069	1.00	26.22
ATOM	2799	N	CYS	365	14.023	56.518	26.290	1.00	25.03
ATOM	2800	CA	CYS	365	14.902	55.370	26.157	1.00	24.77
ATOM	2801	CB	CYS	365	15.450	54.970	27.528	1.00	23.03
ATOM	2802	SG	CYS	365	16.728	56.114	28.173	1.00	21.60
ATOM	2803	C	CYS	365	14.140	54.206	25.514	1.00	26.44
ATOM	2804	O	CYS	365	14.661	53.535	24.617	1.00	27.49
ATOM	2805	N	GLU	366	12.906	53.956	25.944	1.00	26.87
ATOM	2806	CA	GLU	366	12.145	52.859	25.342	1.00	27.98
ATOM	2807	CB	GLU	366	10.757	52.743	25.988	1.00	28.74
ATOM	2808	CG	GLU	366	10.785	52.431	27.490	1.00	30.75
ATOM	2809	CD	GLU	366	9.427	51.981	28.041	1.00	32.09
ATOM	2810	OE1	GLU	366	8.444	52.757	27.970	1.00	32.39
ATOM	2811	OE2	GLU	366	9.342	50.841	28.547	1.00	33.30
ATOM	2812	C	GLU	366	12.005	53.056	23.815	1.00	28.15
ATOM	2813	O	GLU	366	12.117	52.104	23.029	1.00	27.63
ATOM	2814	N	SER	367	11.776	54.304	23.407	1.00	28.42
ATOM	2815	CA	SER	367	11.612	54.650	21.993	1.00	27.23
ATOM	2816	CB	SER	367	11.368	56.156	21.833	1.00	27.45
ATOM	2817	OG	SER	367	10.161	56.552	22.447	1.00	27.44
ATOM	2818	C	SER	367	12.824	54.276	21.165	1.00	26.52
ATOM	2819	O	SER	367	12.724	53.567	20.162	1.00	27.99
ATOM	2820	N	VAL	368	13.977	54.773	21.581	1.00	24.30
ATOM	2821	CA	VAL	368	15.194	54.499	20.849	1.00	22.45
ATOM	2822	CB	VAL	368	16.324	55.395	21.375	1.00	20.96
ATOM	2823	CG1	VAL	368	17.623	55.075	20.682	1.00	18.44
ATOM	2824	CG2	VAL	368	15.928	56.843	21.190	1.00	18.99
ATOM	2825	C	VAL	368	15.605	53.019	20.888	1.00	23.13
ATOM	2826	O	VAL	368	15.850	52.420	19.832	1.00	23.88
ATOM	2827	N	SER	369	15.660	52.405	22.071	1.00	22.54
ATOM	2828	CA	SER	369	16.071	51.003	22.106	1.00	21.93
ATOM	2829	CB	SER	369	16.248	50.476	23.542	1.00	23.39
ATOM	2830	OG	SER	369	15.011	50.251	24.197	1.00	25.91
ATOM	2831	C	SER	369	15.109	50.112	21.348	1.00	20.54
ATOM	2832	O	SER	369	15.526	49.063	20.850	1.00	20.31
ATOM	2833	N	THR	370	13.832	50.499	21.259	1.00	18.40
ATOM	2834	CA	THR	370	12.878	49.682	20.496	1.00	17.32
ATOM	2835	CB	THR	370	11.400	49.976	20.859	1.00	16.46
ATOM	2836	OG1	THR	370	11.053	49.298	22.073	1.00	15.81
ATOM	2837	CG2	THR	370	10.473	49.487	19.774	1.00	14.39
ATOM	2838	C	THR	370	13.076	49.936	19.001	1.00	17.03
ATOM	2839	O	THR	370	12.977	49.008	18.186	1.00	17.38
ATOM	2840	N	ARG	371	13.358	51.177	18.617	1.00	16.71
ATOM	2841	CA	ARG	371	13.562	51.423	17.201	1.00	16.54
ATOM	2842	CB	ARG	371	13.810	52.905	16.882	1.00	17.42
ATOM	2843	CG	ARG	371	14.013	53.123	15.374	1.00	17.76
ATOM	2844	CD	ARG	371	14.283	54.559	14.943	1.00	17.40
ATOM	2845	NE	ARG	371	15.567	55.076	15.412	1.00	18.85
ATOM	2846	CZ	ARG	371	16.159	56.154	14.896	1.00	18.99

FIG. 4XX

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ATOM   2847  NH1 ARG   371      15.583  56.810  13.892  1.00 17.43
ATOM   2848  NH2 ARG   371      17.303  56.605  15.406  1.00 19.19
ATOM   2849  C   ARG   371      14.763  50.607  16.759  1.00 15.91
ATOM   2850  O   ARG   371      14.689  49.929  15.748  1.00 17.14
ATOM   2851  N   ALA   372      15.856  50.644  17.519  1.00 15.40
ATOM   2852  CA  ALA   372      17.061  49.883  17.148  1.00 16.23
ATOM   2853  CB  ALA   372      18.152  50.046  18.197  1.00 15.66
ATOM   2854  C   ALA   372      16.775  48.407  16.957  1.00 16.83
ATOM   2855  O   ALA   372      17.125  47.838  15.923  1.00 18.06
ATOM   2856  N   ALA   373      16.149  47.790  17.955  1.00 16.86
ATOM   2857  CA  ALA   373      15.817  46.367  17.912  1.00 17.10
ATOM   2858  CB  ALA   373      15.027  45.976  19.156  1.00 16.66
ATOM   2859  C   ALA   373      15.024  46.018  16.665  1.00 18.79
ATOM   2860  O   ALA   373      15.301  45.004  16.018  1.00 20.02
ATOM   2861  N   HIS   374      14.037  46.841  16.316  1.00 19.22
ATOM   2862  CA  HIS   374      13.243  46.560  15.122  1.00 20.89
ATOM   2863  CB  HIS   374      12.025  47.489  15.052  1.00 20.98
ATOM   2864  CG  HIS   374      10.948  47.131  16.029  1.00 19.79
ATOM   2865  CD2 HIS   374      10.813  46.065  16.855  1.00 19.53
ATOM   2866  ND1 HIS   374       9.833  47.914  16.229  1.00 19.92
ATOM   2867  CE1 HIS   374       9.057  47.347  17.137  1.00 18.78
ATOM   2868  NE2 HIS   374       9.629  46.223  17.532  1.00 18.61
ATOM   2869  C   HIS   374      14.075  46.696  13.866  1.00 21.57
ATOM   2870  O   HIS   374      14.136  45.789  13.058  1.00 21.42
ATOM   2871  N   MSE   375      14.722  47.835  13.698  1.00 24.00
ATOM   2872  CA  MSE   375      15.561  48.027  12.528  1.00 26.05
ATOM   2873  CB  MSE   375      16.390  49.311  12.666  1.00 28.31
ATOM   2874  CG  MSE   375      15.671  50.558  12.197  1.00 31.46
ATOM   2875  SE  MSE   375      15.246  50.448  10.400  1.00 41.26
ATOM   2876  CE  MSE   375      16.340  51.745   9.680  1.00 36.51
ATOM   2877  C   MSE   375      16.476  46.810  12.390  1.00 25.84
ATOM   2878  O   MSE   375      16.501  46.159  11.351  1.00 26.84
ATOM   2879  N   CYS   376      17.200  46.489  13.455  1.00 25.61
ATOM   2880  CA  CYS   376      18.107  45.349  13.436  1.00 25.11
ATOM   2881  CB  CYS   376      18.693  45.117  14.831  1.00 26.04
ATOM   2882  SG  CYS   376      20.038  43.879  14.876  1.00 27.98
ATOM   2883  C   CYS   376      17.445  44.058  12.931  1.00 24.01
ATOM   2884  O   CYS   376      18.015  43.369  12.078  1.00 24.35
ATOM   2885  N   SER   377      16.251  43.741  13.443  1.00 22.14
ATOM   2886  CA  SER   377      15.519  42.531  13.038  1.00 20.58
ATOM   2887  CB  SER   377      14.203  42.399  13.811  1.00 20.36
ATOM   2888  OG  SER   377      13.233  43.325  13.338  1.00 20.95
ATOM   2889  C   SER   377      15.210  42.535  11.542  1.00 20.00
ATOM   2890  O   SER   377      15.154  41.484  10.900  1.00 19.23
ATOM   2891  N   ALA   378      14.995  43.715  10.980  1.00 19.64
ATOM   2892  CA  ALA   378      14.723  43.787   9.549  1.00 19.32
ATOM   2893  CB  ALA   378      14.521  45.243   9.119  1.00 18.02
ATOM   2894  C   ALA   378      15.958  43.186   8.874  1.00 19.40
ATOM   2895  O   ALA   378      15.860  42.230   8.093  1.00 18.55
ATOM   2896  N   GLY   379      17.123  43.740   9.222  1.00 20.18
ATOM   2897  CA  GLY   379      18.381  43.271   8.669  1.00 20.06
ATOM   2898  C   GLY   379      18.547  41.762   8.734  1.00 19.52
ATOM   2899  O   GLY   379      18.754  41.113   7.704  1.00 20.07
ATOM   2900  N   LEU   380      18.442  41.201   9.936  1.00 18.61
ATOM   2901  CA  LEU   380      18.596  39.763  10.110  1.00 18.74
ATOM   2902  CB  LEU   380      18.489  39.371  11.579  1.00 18.49
ATOM   2903  CG  LEU   380      18.774  37.881  11.816  1.00 17.82
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FIG. 4YY

```
ATOM   2904  CD1 LEU   380      20.215  37.586  11.383  1.00 16.94
ATOM   2905  CD2 LEU   380      18.557  37.512  13.285  1.00 16.34
ATOM   2906  C   LEU   380      17.580  38.938   9.341  1.00 19.56
ATOM   2907  O   LEU   380      17.895  37.833   8.892  1.00 20.67
ATOM   2908  N   ALA   381      16.354  39.447   9.211  1.00 19.83
ATOM   2909  CA  ALA   381      15.311  38.713   8.496  1.00 20.17
ATOM   2910  CB  ALA   381      13.961  39.327   8.759  1.00 19.87
ATOM   2911  C   ALA   381      15.638  38.746   7.009  1.00 21.06
ATOM   2912  O   ALA   381      15.421  37.773   6.269  1.00 21.05
ATOM   2913  N   GLY   382      16.174  39.874   6.567  1.00 21.33
ATOM   2914  CA  GLY   382      16.561  39.965   5.175  1.00 22.63
ATOM   2915  C   GLY   382      17.670  38.954   4.903  1.00 23.10
ATOM   2916  O   GLY   382      17.708  38.319   3.832  1.00 23.74
ATOM   2917  N   VAL   383      18.579  38.778   5.859  1.00 21.83
ATOM   2918  CA  VAL   383      19.642  37.828   5.615  1.00 22.47
ATOM   2919  CB  VAL   383      20.786  37.967   6.643  1.00 22.80
ATOM   2920  CG1 VAL   383      21.737  36.777   6.525  1.00 21.04
ATOM   2921  CG2 VAL   383      21.562  39.298   6.396  1.00 21.85
ATOM   2922  C   VAL   383      19.075  36.423   5.639  1.00 22.92
ATOM   2923  O   VAL   383      19.199  35.681   4.675  1.00 23.65
ATOM   2924  N   ILE   384      18.414  36.061   6.724  1.00 23.52
ATOM   2925  CA  ILE   384      17.853  34.721   6.835  1.00 24.64
ATOM   2926  CB  ILE   384      17.124  34.551   8.179  1.00 24.17
ATOM   2927  CG2 ILE   384      16.533  33.143   8.283  1.00 22.50
ATOM   2928  CG1 ILE   384      18.112  34.810   9.318  1.00 23.69
ATOM   2929  CD1 ILE   384      17.476  34.861  10.661  1.00 24.39
ATOM   2930  C   ILE   384      16.910  34.324   5.691  1.00 26.04
ATOM   2931  O   ILE   384      17.029  33.233   5.144  1.00 26.98
ATOM   2932  N   ASN   385      15.974  35.182   5.310  1.00 26.88
ATOM   2933  CA  ASN   385      15.097  34.785   4.218  1.00 27.99
ATOM   2934  CB  ASN   385      13.984  35.819   3.998  1.00 25.92
ATOM   2935  CG  ASN   385      13.038  35.918   5.174  1.00 23.68
ATOM   2936  OD1 ASN   385      12.721  34.921   5.820  1.00 21.60
ATOM   2937  ND2 ASN   385      12.567  37.128   5.448  1.00 23.03
ATOM   2938  C   ASN   385      15.888  34.579   2.915  1.00 29.62
ATOM   2939  O   ASN   385      15.610  33.647   2.143  1.00 29.62
ATOM   2940  N   ARG   386      16.869  35.440   2.660  1.00 31.30
ATOM   2941  CA  ARG   386      17.660  35.301   1.442  1.00 33.07
ATOM   2942  CB  ARG   386      18.840  36.261   1.446  1.00 32.62
ATOM   2943  CG  ARG   386      19.697  36.147   0.214  1.00 33.28
ATOM   2944  CD  ARG   386      20.908  37.059   0.284  1.00 34.52
ATOM   2945  NE  ARG   386      21.923  36.698  -0.704  1.00 35.29
ATOM   2946  CZ  ARG   386      21.812  36.910  -2.014  1.00 36.32
ATOM   2947  NH1 ARG   386      20.729  37.492  -2.518  1.00 35.95
ATOM   2948  NH2 ARG   386      22.782  36.525  -2.832  1.00 37.07
ATOM   2949  C   ARG   386      18.178  33.875   1.362  1.00 34.69
ATOM   2950  O   ARG   386      18.077  33.232   0.320  1.00 35.70
ATOM   2951  N   MSE   387      18.710  33.383   2.480  1.00 35.94
ATOM   2952  CA  MSE   387      19.250  32.036   2.560  1.00 37.39
ATOM   2953  CB  MSE   387      19.903  31.828   3.927  1.00 39.78
ATOM   2954  CG  MSE   387      21.099  32.754   4.186  1.00 42.37
ATOM   2955  SE  MSE   387      21.873  32.552   5.859  1.00 49.18
ATOM   2956  CE  MSE   387      21.738  30.694   6.097  1.00 44.67
ATOM   2957  C   MSE   387      18.179  30.976   2.311  1.00 38.50
ATOM   2958  O   MSE   387      18.463  29.927   1.721  1.00 37.80
ATOM   2959  N   ARG   388      16.954  31.255   2.769  1.00 40.15
ATOM   2960  CA  ARG   388      15.808  30.352   2.586  1.00 41.28
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FIG. 4ZZ

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ATOM   2961  CB  ARG   388      14.554  30.941   3.245  1.00 42.50
ATOM   2962  CG  ARG   388      13.268  30.115   3.069  1.00 42.73
ATOM   2963  CD  ARG   388      12.266  30.443   4.178  1.00 43.15
ATOM   2964  NE  ARG   388      10.965  29.787   4.012  1.00 44.47
ATOM   2965  CZ  ARG   388      10.049  30.134   3.104  1.00 44.46
ATOM   2966  NH1 ARG   388      10.283  31.139   2.269  1.00 44.11
ATOM   2967  NH2 ARG   388       8.895  29.478   3.033  1.00 44.15
ATOM   2968  C   ARG   388      15.579  30.210   1.094  1.00 41.39
ATOM   2969  O   ARG   388      15.516  29.104   0.554  1.00 40.76
ATOM   2970  N   GLU   389      15.460  31.355   0.439  1.00 41.88
ATOM   2971  CA  GLU   389      15.275  31.405  -0.997  1.00 43.37
ATOM   2972  CB  GLU   389      15.211  32.867  -1.448  1.00 45.21
ATOM   2973  CG  GLU   389      15.227  33.079  -2.957  1.00 48.22
ATOM   2974  CD  GLU   389      13.894  32.754  -3.632  1.00 50.35
ATOM   2975  OE1 GLU   389      13.850  32.799  -4.891  1.00 51.00
ATOM   2976  OE2 GLU   389      12.900  32.464  -2.912  1.00 50.86
ATOM   2977  C   GLU   389      16.476  30.713  -1.635  1.00 43.77
ATOM   2978  O   GLU   389      16.325  29.726  -2.355  1.00 43.53
ATOM   2979  N   SER   390      17.671  31.227  -1.335  1.00 43.84
ATOM   2980  CA  SER   390      18.925  30.697  -1.878  1.00 43.61
ATOM   2981  CB  SER   390      20.112  31.549  -1.425  1.00 43.41
ATOM   2982  OG  SER   390      20.229  32.703  -2.241  1.00 43.45
ATOM   2983  C   SER   390      19.243  29.234  -1.607  1.00 43.62
ATOM   2984  O   SER   390      20.126  28.671  -2.251  1.00 44.11
ATOM   2985  N   ARG   391      18.555  28.614  -0.660  1.00 43.22
ATOM   2986  CA  ARG   391      18.815  27.213  -0.396  1.00 43.67
ATOM   2987  CB  ARG   391      19.174  26.994   1.078  1.00 42.72
ATOM   2988  CG  ARG   391      20.440  27.699   1.512  1.00 41.51
ATOM   2989  CD  ARG   391      20.907  27.245   2.892  1.00 39.51
ATOM   2990  NE  ARG   391      22.183  27.864   3.231  1.00 37.99
ATOM   2991  CZ  ARG   391      22.940  27.512   4.266  1.00 37.81
ATOM   2992  NH1 ARG   391      22.545  26.540   5.070  1.00 36.05
ATOM   2993  NH2 ARG   391      24.105  28.121   4.482  1.00 37.12
ATOM   2994  C   ARG   391      17.578  26.404  -0.756  1.00 44.95
ATOM   2995  O   ARG   391      17.458  25.241  -0.372  1.00 45.05
ATOM   2996  N   SER   392      16.666  27.023  -1.502  1.00 46.71
ATOM   2997  CA  SER   392      15.420  26.367  -1.895  1.00 48.25
ATOM   2998  CB  SER   392      15.631  25.468  -3.121  1.00 48.10
ATOM   2999  OG  SER   392      15.610  26.216  -4.326  1.00 48.60
ATOM   3000  C   SER   392      14.880  25.536  -0.737  1.00 49.61
ATOM   3001  O   SER   392      14.601  24.344  -0.882  1.00 49.37
ATOM   3002  N   GLU   393      14.749  26.175   0.420  1.00 51.58
ATOM   3003  CA  GLU   393      14.237  25.510   1.617  1.00 53.54
ATOM   3004  CB  GLU   393      15.085  25.897   2.842  1.00 54.33
ATOM   3005  CG  GLU   393      16.586  25.655   2.701  1.00 54.92
ATOM   3006  CD  GLU   393      17.057  24.420   3.450  1.00 55.87
ATOM   3007  OE1 GLU   393      16.845  24.347   4.683  1.00 55.29
ATOM   3008  OE2 GLU   393      17.646  23.523   2.806  1.00 56.69
ATOM   3009  C   GLU   393      12.793  25.961   1.838  1.00 54.20
ATOM   3010  O   GLU   393      12.482  27.151   1.693  1.00 53.70
ATOM   3011  N   ASP   394      11.907  25.026   2.173  1.00 55.42
ATOM   3012  CA  ASP   394      10.519  25.404   2.419  1.00 56.88
ATOM   3013  CB  ASP   394       9.585  24.194   2.400  1.00 58.69
ATOM   3014  CG  ASP   394       8.111  24.602   2.415  1.00 61.23
ATOM   3015  OD1 ASP   394       7.691  25.298   3.376  1.00 62.29
ATOM   3016  OD2 ASP   394       7.374  24.237   1.466  1.00 62.03
ATOM   3017  C   ASP   394      10.489  26.041   3.795  1.00 56.57
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FIG. 4AAA

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ATOM   3018  O   ASP  394      10.023  27.164   3.959  1.00 56.22
ATOM   3019  N   VAL  395      10.994  25.298   4.773  1.00 56.79
ATOM   3020  CA  VAL  395      11.086  25.756   6.153  1.00 57.23
ATOM   3021  CB  VAL  395      10.166  24.949   7.093  1.00 57.72
ATOM   3022  CG1 VAL  395      10.444  25.320   8.548  1.00 57.64
ATOM   3023  CG2 VAL  395       8.708  25.221   6.749  1.00 58.46
ATOM   3024  C   VAL  395      12.534  25.538   6.575  1.00 57.01
ATOM   3025  O   VAL  395      12.968  24.407   6.793  1.00 56.90
ATOM   3026  N   MSE  396      13.280  26.626   6.690  1.00 56.80
ATOM   3027  CA  MSE  396      14.682  26.536   7.058  1.00 56.12
ATOM   3028  CB  MSE  396      15.463  27.645   6.375  1.00 57.66
ATOM   3029  CG  MSE  396      16.932  27.623   6.690  1.00 60.51
ATOM   3030  SE  MSE  396      17.716  29.077   6.002  1.00 65.26
ATOM   3031  CE  MSE  396      17.988  28.564   4.293  1.00 64.74
ATOM   3032  C   MSE  396      14.964  26.600   8.545  1.00 54.59
ATOM   3033  O   MSE  396      14.487  27.491   9.245  1.00 54.08
ATOM   3034  N   ARG  397      15.740  25.637   9.025  1.00 53.05
ATOM   3035  CA  ARG  397      16.134  25.613  10.426  1.00 51.13
ATOM   3036  CB  ARG  397      16.226  24.181  10.951  1.00 52.77
ATOM   3037  CG  ARG  397      14.888  23.520  11.244  1.00 55.36
ATOM   3038  CD  ARG  397      15.132  22.079  11.671  1.00 58.69
ATOM   3039  NE  ARG  397      13.985  21.448  12.326  1.00 61.28
ATOM   3040  CZ  ARG  397      14.056  20.294  12.990  1.00 62.10
ATOM   3041  NH1 ARG  397      15.215  19.651  13.078  1.00 62.57
ATOM   3042  NH2 ARG  397      12.978  19.793  13.583  1.00 62.49
ATOM   3043  C   ARG  397      17.509  26.252  10.397  1.00 48.33
ATOM   3044  O   ARG  397      18.273  26.029   9.466  1.00 47.77
ATOM   3045  N   ILE  398      17.825  27.064  11.395  1.00 45.82
ATOM   3046  CA  ILE  398      19.120  27.721  11.396  1.00 43.01
ATOM   3047  CB  ILE  398      19.202  28.791  10.293  1.00 43.25
ATOM   3048  CG2 ILE  398      18.161  29.864  10.532  1.00 43.18
ATOM   3049  CG1 ILE  398      20.594  29.417  10.279  1.00 43.75
ATOM   3050  CD1 ILE  398      20.768  30.466   9.206  1.00 44.64
ATOM   3051  C   ILE  398      19.441  28.381  12.717  1.00 40.64
ATOM   3052  O   ILE  398      18.557  28.890  13.404  1.00 40.10
ATOM   3053  N   THR  399      20.722  28.360  13.060  1.00 37.78
ATOM   3054  CA  THR  399      21.185  28.954  14.290  1.00 35.36
ATOM   3055  CB  THR  399      22.052  27.988  15.079  1.00 35.02
ATOM   3056  OG1 THR  399      21.280  26.832  15.425  1.00 34.92
ATOM   3057  CG2 THR  399      22.570  28.666  16.345  1.00 34.73
ATOM   3058  C   THR  399      22.001  30.197  13.994  1.00 34.71
ATOM   3059  O   THR  399      22.736  30.254  13.005  1.00 35.10
ATOM   3060  N   VAL  400      21.858  31.184  14.871  1.00 32.96
ATOM   3061  CA  VAL  400      22.539  32.457  14.759  1.00 31.07
ATOM   3062  CB  VAL  400      21.514  33.593  14.592  1.00 31.21
ATOM   3063  CG1 VAL  400      22.211  34.934  14.415  1.00 31.76
ATOM   3064  CG2 VAL  400      20.628  33.298  13.405  1.00 31.47
ATOM   3065  C   VAL  400      23.336  32.685  16.039  1.00 30.19
ATOM   3066  O   VAL  400      22.779  32.640  17.144  1.00 30.96
ATOM   3067  N   GLY  401      24.641  32.905  15.888  1.00 28.35
ATOM   3068  CA  GLY  401      25.482  33.150  17.041  1.00 24.47
ATOM   3069  C   GLY  401      25.487  34.641  17.235  1.00 23.04
ATOM   3070  O   GLY  401      25.595  35.388  16.260  1.00 20.38
ATOM   3071  N   VAL  402      25.367  35.086  18.482  1.00 23.36
ATOM   3072  CA  VAL  402      25.338  36.514  18.751  1.00 23.38
ATOM   3073  CB  VAL  402      23.927  36.960  19.124  1.00 22.79
ATOM   3074  CG1 VAL  402      23.790  38.458  18.909  1.00 22.85
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FIG. 4BBB

ATOM	3075	CG2	VAL	402	22.895	36.176	18.320	1.00	22.42
ATOM	3076	C	VAL	402	26.252	36.899	19.893	1.00	24.25
ATOM	3077	O	VAL	402	26.484	36.098	20.794	1.00	25.20
ATOM	3078	N	ASP	403	26.770	38.124	19.848	1.00	24.83
ATOM	3079	CA	ASP	403	27.637	38.649	20.894	1.00	27.11
ATOM	3080	CB	ASP	403	29.078	38.212	20.691	1.00	30.98
ATOM	3081	CG	ASP	403	30.003	38.739	21.787	1.00	34.48
ATOM	3082	OD1	ASP	403	29.887	39.938	22.122	1.00	36.02
ATOM	3083	OD2	ASP	403	30.842	37.960	22.311	1.00	36.05
ATOM	3084	C	ASP	403	27.562	40.154	20.763	1.00	27.24
ATOM	3085	O	ASP	403	27.550	40.667	19.645	1.00	29.15
ATOM	3086	N	GLY	404	27.519	40.863	21.888	1.00	26.60
ATOM	3087	CA	GLY	404	27.410	42.316	21.863	1.00	26.50
ATOM	3088	C	GLY	404	26.750	42.829	23.137	1.00	27.10
ATOM	3089	O	GLY	404	25.810	42.193	23.665	1.00	26.90
ATOM	3090	N	SER	405	27.209	43.972	23.644	1.00	26.72
ATOM	3091	CA	SER	405	26.638	44.496	24.887	1.00	27.96
ATOM	3092	CB	SER	405	27.409	45.722	25.371	1.00	28.04
ATOM	3093	OG	SER	405	27.164	46.828	24.521	1.00	30.53
ATOM	3094	C	SER	405	25.168	44.857	24.738	1.00	28.25
ATOM	3095	O	SER	405	24.341	44.473	25.573	1.00	27.96
ATOM	3096	N	VAL	406	24.844	45.591	23.675	1.00	27.79
ATOM	3097	CA	VAL	406	23.465	45.992	23.445	1.00	28.13
ATOM	3098	CB	VAL	406	23.281	46.667	22.074	1.00	28.02
ATOM	3099	CG1	VAL	406	21.814	47.063	21.908	1.00	27.91
ATOM	3100	CG2	VAL	406	24.197	47.877	21.940	1.00	26.07
ATOM	3101	C	VAL	406	22.535	44.789	23.488	1.00	28.35
ATOM	3102	O	VAL	406	21.484	44.826	24.120	1.00	28.48
ATOM	3103	N	TYR	407	22.934	43.718	22.811	1.00	28.72
ATOM	3104	CA	TYR	407	22.130	42.493	22.736	1.00	28.45
ATOM	3105	CB	TYR	407	22.613	41.643	21.558	1.00	26.86
ATOM	3106	CG	TYR	407	21.831	40.373	21.341	1.00	25.29
ATOM	3107	CD1	TYR	407	20.700	40.358	20.535	1.00	25.44
ATOM	3108	CE1	TYR	407	19.964	39.189	20.346	1.00	25.93
ATOM	3109	CD2	TYR	407	22.213	39.192	21.955	1.00	24.93
ATOM	3110	CE2	TYR	407	21.488	38.021	21.780	1.00	25.18
ATOM	3111	CZ	TYR	407	20.362	38.024	20.974	1.00	26.03
ATOM	3112	OH	TYR	407	19.626	36.868	20.822	1.00	25.67
ATOM	3113	C	TYR	407	22.175	41.651	24.014	1.00	28.83
ATOM	3114	O	TYR	407	21.202	40.988	24.369	1.00	28.62
ATOM	3115	N	LYS	408	23.306	41.674	24.705	1.00	29.64
ATOM	3116	CA	LYS	408	23.440	40.881	25.916	1.00	30.07
ATOM	3117	CB	LYS	408	24.904	40.477	26.118	1.00	30.08
ATOM	3118	CG	LYS	408	25.442	39.556	25.030	1.00	30.61
ATOM	3119	CD	LYS	408	26.597	38.698	25.529	1.00	30.05
ATOM	3120	CE	LYS	408	26.799	37.515	24.601	1.00	30.22
ATOM	3121	NZ	LYS	408	27.828	36.573	25.097	1.00	30.20
ATOM	3122	C	LYS	408	22.940	41.551	27.185	1.00	30.82
ATOM	3123	O	LYS	408	22.327	40.901	28.038	1.00	31.98
ATOM	3124	N	LEU	409	23.176	42.853	27.296	1.00	30.97
ATOM	3125	CA	LEU	409	22.823	43.598	28.501	1.00	31.11
ATOM	3126	CB	LEU	409	24.006	44.482	28.875	1.00	30.54
ATOM	3127	CG	LEU	409	25.305	43.700	28.962	1.00	29.31
ATOM	3128	CD1	LEU	409	26.372	44.591	29.597	1.00	29.41
ATOM	3129	CD2	LEU	409	25.067	42.423	29.785	1.00	28.16
ATOM	3130	C	LEU	409	21.548	44.441	28.611	1.00	31.44
ATOM	3131	O	LEU	409	20.978	44.542	29.708	1.00	31.86

FIG. 4CCC

```
ATOM   3132  N   HIS  410      21.122  45.077  27.519  1.00 31.34
ATOM   3133  CA  HIS  410      19.929  45.912  27.572  1.00 30.80
ATOM   3134  CB  HIS  410      19.732  46.635  26.247  1.00 30.36
ATOM   3135  CG  HIS  410      18.703  47.717  26.303  1.00 29.89
ATOM   3136  CD2 HIS  410      18.815  49.060  26.179  1.00 29.29
ATOM   3137  ND1 HIS  410      17.362  47.457  26.508  1.00 30.79
ATOM   3138  CE1 HIS  410      16.691  48.595  26.505  1.00 29.88
ATOM   3139  NE2 HIS  410      17.548  49.583  26.309  1.00 30.87
ATOM   3140  C   HIS  410      18.728  45.031  27.900  1.00 31.41
ATOM   3141  O   HIS  410      18.467  44.055  27.207  1.00 31.97
ATOM   3142  N   PRO  411      17.985  45.376  28.969  1.00 31.63
ATOM   3143  CD  PRO  411      18.173  46.690  29.610  1.00 31.32
ATOM   3144  CA  PRO  411      16.798  44.708  29.518  1.00 31.33
ATOM   3145  CB  PRO  411      16.111  45.815  30.299  1.00 31.27
ATOM   3146  CG  PRO  411      17.257  46.599  30.822  1.00 32.32
ATOM   3147  C   PRO  411      15.827  44.037  28.571  1.00 32.09
ATOM   3148  O   PRO  411      15.362  42.920  28.838  1.00 32.76
ATOM   3149  N   SER  412      15.519  44.684  27.457  1.00 31.73
ATOM   3150  CA  SER  412      14.527  44.094  26.573  1.00 31.92
ATOM   3151  CB  SER  412      13.210  44.834  26.771  1.00 32.51
ATOM   3152  OG  SER  412      13.368  46.200  26.390  1.00 33.27
ATOM   3153  C   SER  412      14.838  44.047  25.082  1.00 31.91
ATOM   3154  O   SER  412      14.039  43.520  24.304  1.00 32.59
ATOM   3155  N   PHE  413      15.974  44.601  24.679  1.00 30.72
ATOM   3156  CA  PHE  413      16.348  44.615  23.271  1.00 30.13
ATOM   3157  CB  PHE  413      17.778  45.105  23.130  1.00 28.18
ATOM   3158  CG  PHE  413      18.213  45.285  21.716  1.00 25.96
ATOM   3159  CD1 PHE  413      18.085  46.522  21.094  1.00 25.70
ATOM   3160  CD2 PHE  413      18.772  44.233  21.015  1.00 24.47
ATOM   3161  CE1 PHE  413      18.517  46.711  19.787  1.00 25.13
ATOM   3162  CE2 PHE  413      19.208  44.408  19.707  1.00 24.84
ATOM   3163  CZ  PHE  413      19.082  45.652  19.092  1.00 24.48
ATOM   3164  C   PHE  413      16.232  43.228  22.645  1.00 31.20
ATOM   3165  O   PHE  413      15.571  43.026  21.612  1.00 31.56
ATOM   3166  N   LYS  414      16.888  42.268  23.275  1.00 31.75
ATOM   3167  CA  LYS  414      16.851  40.906  22.790  1.00 32.75
ATOM   3168  CB  LYS  414      17.626  39.999  23.755  1.00 33.66
ATOM   3169  CG  LYS  414      17.570  38.526  23.429  1.00 34.45
ATOM   3170  CD  LYS  414      18.732  37.744  24.049  1.00 36.05
ATOM   3171  CE  LYS  414      18.845  37.909  25.558  1.00 35.80
ATOM   3172  NZ  LYS  414      19.972  38.817  25.920  1.00 36.66
ATOM   3173  C   LYS  414      15.412  40.411  22.600  1.00 33.19
ATOM   3174  O   LYS  414      15.054  39.927  21.518  1.00 33.30
ATOM   3175  N   GLU  415      14.577  40.542  23.627  1.00 33.81
ATOM   3176  CA  GLU  415      13.193  40.071  23.513  1.00 34.53
ATOM   3177  CB  GLU  415      12.462  40.251  24.838  1.00 37.66
ATOM   3178  CG  GLU  415      13.062  39.497  26.002  1.00 42.83
ATOM   3179  CD  GLU  415      14.376  40.090  26.520  1.00 45.68
ATOM   3180  OE1 GLU  415      14.523  41.339  26.526  1.00 47.31
ATOM   3181  OE2 GLU  415      15.245  39.293  26.956  1.00 47.44
ATOM   3182  C   GLU  415      12.409  40.776  22.401  1.00 33.23
ATOM   3183  O   GLU  415      11.676  40.137  21.649  1.00 33.06
ATOM   3184  N   ARG  416      12.551  42.092  22.299  1.00 31.77
ATOM   3185  CA  ARG  416      11.841  42.825  21.264  1.00 30.32
ATOM   3186  CB  ARG  416      12.066  44.328  21.427  1.00 31.27
ATOM   3187  CG  ARG  416      11.645  44.875  22.796  1.00 33.92
ATOM   3188  CD  ARG  416      11.783  46.393  22.901  1.00 35.48
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FIG. 4DDD

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ATOM   3189  NE  ARG   416      11.545  46.866  24.267  1.00 38.24
ATOM   3190  CZ  ARG   416      11.982  48.030  24.746  1.00 39.11
ATOM   3191  NH1 ARG   416      12.676  48.850  23.967  1.00 39.89
ATOM   3192  NH2 ARG   416      11.754  48.365  26.009  1.00 38.52
ATOM   3193  C   ARG   416      12.379  42.354  19.916  1.00 29.08
ATOM   3194  O   ARG   416      11.620  42.159  18.964  1.00 28.85
ATOM   3195  N   PHE   417      13.694  42.144  19.862  1.00 27.59
ATOM   3196  CA  PHE   417      14.377  41.707  18.648  1.00 25.70
ATOM   3197  CB  PHE   417      15.886  41.687  18.890  1.00 23.64
ATOM   3198  CG  PHE   417      16.687  41.310  17.680  1.00 20.59
ATOM   3199  CD1 PHE   417      16.910  42.230  16.671  1.00 18.99
ATOM   3200  CD2 PHE   417      17.183  40.018  17.540  1.00 19.41
ATOM   3201  CE1 PHE   417      17.610  41.870  15.540  1.00 19.87
ATOM   3202  CE2 PHE   417      17.884  39.641  16.413  1.00 18.04
ATOM   3203  CZ  PHE   417      18.100  40.563  15.409  1.00 20.04
ATOM   3204  C   PHE   417      13.943  40.342  18.099  1.00 25.74
ATOM   3205  O   PHE   417      13.568  40.225  16.927  1.00 25.24
ATOM   3206  N   HIS   418      14.012  39.301  18.922  1.00 26.11
ATOM   3207  CA  HIS   418      13.612  37.962  18.459  1.00 26.79
ATOM   3208  CB  HIS   418      13.638  36.973  19.615  1.00 28.01
ATOM   3209  CG  HIS   418      14.973  36.854  20.279  1.00 28.81
ATOM   3210  CD2 HIS   418      16.168  37.425  19.989  1.00 29.42
ATOM   3211  ND1 HIS   418      15.182  36.067  21.389  1.00 28.15
ATOM   3212  CE1 HIS   418      16.446  36.157  21.755  1.00 29.43
ATOM   3213  NE2 HIS   418      17.067  36.974  20.924  1.00 29.74
ATOM   3214  C   HIS   418      12.209  37.985  17.876  1.00 26.41
ATOM   3215  O   HIS   418      11.976  37.565  16.733  1.00 26.40
ATOM   3216  N   ALA   419      11.284  38.487  18.688  1.00 25.83
ATOM   3217  CA  ALA   419       9.885  38.603  18.328  1.00 25.05
ATOM   3218  CB  ALA   419       9.182  39.454  19.352  1.00 24.80
ATOM   3219  C   ALA   419       9.731  39.215  16.943  1.00 25.35
ATOM   3220  O   ALA   419       9.146  38.601  16.029  1.00 25.99
ATOM   3221  N   SER   420      10.249  40.425  16.777  1.00 25.26
ATOM   3222  CA  SER   420      10.159  41.078  15.481  1.00 25.31
ATOM   3223  CB  SER   420      10.897  42.405  15.515  1.00 23.85
ATOM   3224  OG  SER   420      10.692  43.089  14.303  1.00 23.43
ATOM   3225  C   SER   420      10.751  40.170  14.391  1.00 26.14
ATOM   3226  O   SER   420      10.145  39.976  13.331  1.00 25.95
ATOM   3227  N   VAL   421      11.926  39.602  14.670  1.00 27.34
ATOM   3228  CA  VAL   421      12.602  38.699  13.733  1.00 28.41
ATOM   3229  CB  VAL   421      13.919  38.127  14.346  1.00 27.63
ATOM   3230  CG1 VAL   421      14.479  37.020  13.475  1.00 26.36
ATOM   3231  CG2 VAL   421      14.953  39.232  14.469  1.00 28.22
ATOM   3232  C   VAL   421      11.689  37.535  13.325  1.00 29.65
ATOM   3233  O   VAL   421      11.557  37.227  12.130  1.00 28.72
ATOM   3234  N   ARG   422      11.069  36.886  14.310  1.00 30.74
ATOM   3235  CA  ARG   422      10.165  35.775  14.014  1.00 32.79
ATOM   3236  CB  ARG   422       9.419  35.328  15.265  1.00 33.29
ATOM   3237  CG  ARG   422      10.259  35.197  16.512  1.00 34.47
ATOM   3238  CD  ARG   422      11.081  33.927  16.558  1.00 34.54
ATOM   3239  NE  ARG   422      11.862  33.905  17.795  1.00 35.75
ATOM   3240  CZ  ARG   422      12.824  33.028  18.066  1.00 35.45
ATOM   3241  NH1 ARG   422      13.127  32.085  17.180  1.00 35.35
ATOM   3242  NH2 ARG   422      13.490  33.108  19.215  1.00 33.55
ATOM   3243  C   ARG   422       9.123  36.277  13.019  1.00 33.41
ATOM   3244  O   ARG   422       8.949  35.728  11.929  1.00 33.68
ATOM   3245  N   ARG   423       8.446  37.348  13.417  1.00 34.00
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FIG. 4EEE

ATOM	3246	CA	ARG	423	7.394	37.946	12.622	1.00	34.13
ATOM	3247	CB	ARG	423	7.022	39.301	13.207	1.00	35.16
ATOM	3248	CG	ARG	423	5.538	39.584	13.202	1.00	36.10
ATOM	3249	CD	ARG	423	5.212	40.831	14.012	1.00	37.57
ATOM	3250	NE	ARG	423	5.482	40.682	15.441	1.00	38.90
ATOM	3251	CZ	ARG	423	6.274	41.503	16.133	1.00	40.51
ATOM	3252	NH1	ARG	423	6.874	42.523	15.513	1.00	41.42
ATOM	3253	NH2	ARG	423	6.461	41.324	17.440	1.00	38.76
ATOM	3254	C	ARG	423	7.754	38.100	11.165	1.00	33.94
ATOM	3255	O	ARG	423	6.919	37.849	10.295	1.00	35.59
ATOM	3256	N	LEU	424	8.993	38.494	10.884	1.00	32.85
ATOM	3257	CA	LEU	424	9.418	38.699	9.497	1.00	31.57
ATOM	3258	CB	LEU	424	10.474	39.788	9.450	1.00	28.75
ATOM	3259	CG	LEU	424	10.030	41.129	10.003	1.00	27.64
ATOM	3260	CD1	LEU	424	11.220	42.080	10.066	1.00	26.47
ATOM	3261	CD2	LEU	424	8.942	41.686	9.115	1.00	27.23
ATOM	3262	C	LEU	424	9.950	37.479	8.747	1.00	32.00
ATOM	3263	O	LEU	424	10.232	37.562	7.551	1.00	31.15
ATOM	3264	N	THR	425	10.065	36.343	9.424	1.00	33.88
ATOM	3265	CA	THR	425	10.615	35.153	8.778	1.00	35.30
ATOM	3266	CB	THR	425	11.886	34.722	9.495	1.00	35.17
ATOM	3267	OG1	THR	425	11.580	34.463	10.874	1.00	35.24
ATOM	3268	CG2	THR	425	12.939	35.817	9.399	1.00	35.16
ATOM	3269	C	THR	425	9.711	33.923	8.675	1.00	37.00
ATOM	3270	O	THR	425	10.059	32.854	9.182	1.00	37.54
ATOM	3271	N	PRO	426	8.562	34.040	7.982	1.00	38.04
ATOM	3272	CD	PRO	426	8.144	35.123	7.073	1.00	38.49
ATOM	3273	CA	PRO	426	7.663	32.890	7.856	1.00	38.85
ATOM	3274	CB	PRO	426	6.745	33.295	6.700	1.00	38.23
ATOM	3275	CG	PRO	426	6.699	34.772	6.802	1.00	38.07
ATOM	3276	C	PRO	426	8.445	31.615	7.527	1.00	39.83
ATOM	3277	O	PRO	426	9.378	31.641	6.728	1.00	40.28
ATOM	3278	N	SER	427	8.073	30.510	8.158	1.00	40.72
ATOM	3279	CA	SER	427	8.713	29.232	7.892	1.00	41.82
ATOM	3280	CB	SER	427	8.358	28.785	6.474	1.00	42.86
ATOM	3281	OG	SER	427	6.954	28.802	6.287	1.00	44.69
ATOM	3282	C	SER	427	10.234	29.228	8.068	1.00	42.10
ATOM	3283	O	SER	427	10.981	28.899	7.140	1.00	41.85
ATOM	3284	N	CYS	428	10.679	29.586	9.267	1.00	42.60
ATOM	3285	CA	CYS	428	12.096	29.608	9.601	1.00	42.43
ATOM	3286	CB	CYS	428	12.724	30.960	9.258	1.00	42.59
ATOM	3287	SG	CYS	428	12.860	31.327	7.492	1.00	44.02
ATOM	3288	C	CYS	428	12.195	29.381	11.096	1.00	42.45
ATOM	3289	O	CYS	428	11.671	30.169	11.879	1.00	43.76
ATOM	3290	N	GLU	429	12.846	28.296	11.494	1.00	42.34
ATOM	3291	CA	GLU	429	13.014	27.995	12.909	1.00	41.23
ATOM	3292	CB	GLU	429	13.030	26.486	13.146	1.00	42.97
ATOM	3293	CG	GLU	429	11.699	25.796	12.933	1.00	45.48
ATOM	3294	CD	GLU	429	11.847	24.282	12.925	1.00	47.43
ATOM	3295	OE1	GLU	429	12.518	23.756	13.847	1.00	48.77
ATOM	3296	OE2	GLU	429	11.298	23.623	12.005	1.00	48.07
ATOM	3297	C	GLU	429	14.341	28.587	13.346	1.00	39.77
ATOM	3298	O	GLU	429	15.370	27.902	13.352	1.00	39.92
ATOM	3299	N	ILE	430	14.315	29.864	13.708	1.00	38.09
ATOM	3300	CA	ILE	430	15.514	30.560	14.142	1.00	36.48
ATOM	3301	CB	ILE	430	15.341	32.070	13.998	1.00	35.17
ATOM	3302	CG2	ILE	430	16.659	32.770	14.280	1.00	34.48

FIG. 4FFF

ATOM	3303	CG1	ILE	430	14.839	32.390	12.589	1.00	35.30
ATOM	3304	CD1	ILE	430	14.669	33.866	12.310	1.00	34.88
ATOM	3305	C	ILE	430	15.872	30.254	15.591	1.00	37.06
ATOM	3306	O	ILE	430	15.044	30.399	16.495	1.00	38.13
ATOM	3307	N	THR	431	17.109	29.823	15.808	1.00	36.61
ATOM	3308	CA	THR	431	17.600	29.520	17.146	1.00	36.17
ATOM	3309	CB	THR	431	18.067	28.053	17.240	1.00	36.58
ATOM	3310	OG1	THR	431	16.950	27.180	17.031	1.00	36.34
ATOM	3311	CG2	THR	431	18.692	27.774	18.604	1.00	36.38
ATOM	3312	C	THR	431	18.796	30.441	17.396	1.00	36.13
ATOM	3313	O	THR	431	19.705	30.513	16.569	1.00	36.10
ATOM	3314	N	PHE	432	18.804	31.157	18.514	1.00	35.79
ATOM	3315	CA	PHE	432	19.926	32.054	18.794	1.00	35.93
ATOM	3316	CB	PHE	432	19.443	33.450	19.232	1.00	34.31
ATOM	3317	CG	PHE	432	18.643	34.194	18.188	1.00	32.53
ATOM	3318	CD1	PHE	432	17.271	33.977	18.048	1.00	31.59
ATOM	3319	CD2	PHE	432	19.262	35.124	17.353	1.00	31.00
ATOM	3320	CE1	PHE	432	16.527	34.676	17.092	1.00	30.53
ATOM	3321	CE2	PHE	432	18.525	35.826	16.395	1.00	30.25
ATOM	3322	CZ	PHE	432	17.154	35.600	16.266	1.00	30.11
ATOM	3323	C	PHE	432	20.767	31.483	19.917	1.00	37.08
ATOM	3324	O	PHE	432	20.248	30.772	20.779	1.00	38.85
ATOM	3325	N	ILE	433	22.063	31.774	19.906	1.00	37.32
ATOM	3326	CA	ILE	433	22.933	31.321	20.983	1.00	38.46
ATOM	3327	CB	ILE	433	23.526	29.890	20.722	1.00	39.06
ATOM	3328	CG2	ILE	433	22.398	28.863	20.624	1.00	38.62
ATOM	3329	CG1	ILE	433	24.367	29.861	19.449	1.00	39.03
ATOM	3330	CD1	ILE	433	25.028	28.520	19.227	1.00	38.32
ATOM	3331	C	ILE	433	24.039	32.358	21.161	1.00	39.33
ATOM	3332	O	ILE	433	24.429	33.034	20.201	1.00	39.15
ATOM	3333	N	GLU	434	24.527	32.505	22.388	1.00	40.58
ATOM	3334	CA	GLU	434	25.559	33.498	22.669	1.00	42.92
ATOM	3335	CB	GLU	434	25.152	34.312	23.885	1.00	43.91
ATOM	3336	CG	GLU	434	23.769	34.883	23.744	1.00	45.53
ATOM	3337	CD	GLU	434	23.342	35.640	24.965	1.00	46.68
ATOM	3338	OE1	GLU	434	23.436	35.072	26.074	1.00	47.18
ATOM	3339	OE2	GLU	434	22.910	36.802	24.816	1.00	48.77
ATOM	3340	C	GLU	434	26.965	32.950	22.865	1.00	44.01
ATOM	3341	O	GLU	434	27.206	32.058	23.680	1.00	44.48
ATOM	3342	N	SER	435	27.901	33.518	22.119	1.00	45.00
ATOM	3343	CA	SER	435	29.284	33.075	22.167	1.00	46.11
ATOM	3344	CB	SER	435	30.077	33.779	21.057	1.00	46.95
ATOM	3345	OG	SER	435	29.839	35.186	21.053	1.00	47.94
ATOM	3346	C	SER	435	29.984	33.274	23.507	1.00	46.36
ATOM	3347	O	SER	435	30.043	34.396	24.022	1.00	46.31
ATOM	3348	N	GLU	436	30.505	32.180	24.069	1.00	46.22
ATOM	3349	CA	GLU	436	31.248	32.250	25.330	1.00	46.33
ATOM	3350	CB	GLU	436	31.322	30.884	26.020	1.00	47.64
ATOM	3351	CG	GLU	436	32.144	30.908	27.317	1.00	50.83
ATOM	3352	CD	GLU	436	32.726	29.541	27.711	1.00	52.03
ATOM	3353	OE1	GLU	436	31.951	28.585	27.970	1.00	52.84
ATOM	3354	OE2	GLU	436	33.972	29.428	27.765	1.00	52.07
ATOM	3355	C	GLU	436	32.650	32.671	24.912	1.00	45.58
ATOM	3356	O	GLU	436	33.446	31.843	24.463	1.00	45.50
ATOM	3357	N	GLU	437	32.950	33.956	25.051	1.00	44.67
ATOM	3358	CA	GLU	437	34.252	34.462	24.643	1.00	44.13
ATOM	3359	CB	GLU	437	35.328	34.050	25.652	1.00	43.61

FIG. 4GGG

ATOM	3360	CG	GLU	437	36.745	34.334	25.190	1.00	43.39
ATOM	3361	CD	GLU	437	36.931	35.752	24.678	1.00	43.50
ATOM	3362	OE1	GLU	437	36.976	36.680	25.514	1.00	44.49
ATOM	3363	OE2	GLU	437	37.025	35.940	23.441	1.00	42.17
ATOM	3364	C	GLU	437	34.569	33.880	23.264	1.00	43.56
ATOM	3365	O	GLU	437	35.530	33.131	23.108	1.00	45.30
ATOM	3366	N	GLY	438	33.757	34.225	22.266	1.00	41.68
ATOM	3367	CA	GLY	438	33.958	33.700	20.926	1.00	39.44
ATOM	3368	C	GLY	438	34.748	34.538	19.934	1.00	38.11
ATOM	3369	O	GLY	438	34.932	34.130	18.791	1.00	37.45
ATOM	3370	N	SER	439	35.213	35.713	20.329	1.00	37.14
ATOM	3371	CA	SER	439	35.980	36.502	19.386	1.00	36.86
ATOM	3372	CB	SER	439	35.916	37.983	19.714	1.00	36.81
ATOM	3373	OG	SER	439	36.825	38.678	18.878	1.00	35.32
ATOM	3374	C	SER	439	37.420	36.053	19.444	1.00	36.74
ATOM	3375	O	SER	439	38.192	36.265	18.513	1.00	36.37
ATOM	3376	N	GLY	440	37.774	35.439	20.562	1.00	36.58
ATOM	3377	CA	GLY	440	39.126	34.957	20.746	1.00	36.42
ATOM	3378	C	GLY	440	39.207	33.518	20.302	1.00	36.28
ATOM	3379	O	GLY	440	40.146	33.140	19.613	1.00	36.20
ATOM	3380	N	ARG	441	38.224	32.714	20.699	1.00	36.09
ATOM	3381	CA	ARG	441	38.190	31.309	20.312	1.00	37.16
ATOM	3382	CB	ARG	441	37.151	30.562	21.138	1.00	37.34
ATOM	3383	CG	ARG	441	37.312	30.717	22.632	1.00	39.57
ATOM	3384	CD	ARG	441	36.334	29.806	23.375	1.00	42.28
ATOM	3385	NE	ARG	441	35.270	29.339	22.488	1.00	44.36
ATOM	3386	CZ	ARG	441	34.240	28.585	22.862	1.00	45.80
ATOM	3387	NH1	ARG	441	34.103	28.192	24.127	1.00	45.87
ATOM	3388	NH2	ARG	441	33.346	28.214	21.955	1.00	47.26
ATOM	3389	C	ARG	441	37.848	31.179	18.821	1.00	37.42
ATOM	3390	O	ARG	441	38.103	30.151	18.189	1.00	37.52
ATOM	3391	N	GLY	442	37.270	32.234	18.262	1.00	37.34
ATOM	3392	CA	GLY	442	36.906	32.204	16.863	1.00	37.39
ATOM	3393	C	GLY	442	38.165	32.308	16.048	1.00	37.47
ATOM	3394	O	GLY	442	38.483	31.410	15.278	1.00	37.51
ATOM	3395	N	ALA	443	38.887	33.408	16.241	1.00	38.17
ATOM	3396	CA	ALA	443	40.134	33.660	15.526	1.00	38.50
ATOM	3397	CB	ALA	443	40.739	34.999	15.967	1.00	36.50
ATOM	3398	C	ALA	443	41.127	32.521	15.759	1.00	39.03
ATOM	3399	O	ALA	443	42.015	32.297	14.941	1.00	39.36
ATOM	3400	N	ALA	444	40.977	31.807	16.875	1.00	39.93
ATOM	3401	CA	ALA	444	41.864	30.685	17.172	1.00	40.31
ATOM	3402	CB	ALA	444	41.724	30.242	18.623	1.00	39.25
ATOM	3403	C	ALA	444	41.427	29.569	16.246	1.00	40.97
ATOM	3404	O	ALA	444	42.146	29.210	15.312	1.00	41.31
ATOM	3405	N	LEU	445	40.233	29.038	16.501	1.00	41.41
ATOM	3406	CA	LEU	445	39.678	27.960	15.690	1.00	41.97
ATOM	3407	CB	LEU	445	38.195	27.776	16.024	1.00	40.09
ATOM	3408	CG	LEU	445	37.954	26.806	17.182	1.00	39.14
ATOM	3409	CD1	LEU	445	36.750	27.233	17.982	1.00	39.27
ATOM	3410	CD2	LEU	445	37.781	25.399	16.647	1.00	37.36
ATOM	3411	C	LEU	445	39.860	28.156	14.176	1.00	43.29
ATOM	3412	O	LEU	445	39.918	27.179	13.427	1.00	43.28
ATOM	3413	N	VAL	446	39.955	29.406	13.729	1.00	44.66
ATOM	3414	CA	VAL	446	40.136	29.684	12.307	1.00	46.32
ATOM	3415	CB	VAL	446	39.687	31.120	11.948	1.00	46.15
ATOM	3416	CG1	VAL	446	40.356	31.578	10.653	1.00	46.15

FIG. 4HHH

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ATOM   3417  CG2 VAL   446      38.164  31.160  11.793  1.00 45.75
ATOM   3418  C   VAL   446      41.597  29.503  11.944  1.00 48.03
ATOM   3419  O   VAL   446      41.929  29.105  10.825  1.00 48.75
ATOM   3420  N   SER   447      42.465  29.802  12.904  1.00 49.63
ATOM   3421  CA  SER   447      43.902  29.657  12.725  1.00 50.76
ATOM   3422  CB  SER   447      44.635  30.267  13.918  1.00 50.76
ATOM   3423  OG  SER   447      44.377  31.659  14.021  1.00 50.83
ATOM   3424  C   SER   447      44.259  28.173  12.612  1.00 52.07
ATOM   3425  O   SER   447      44.923  27.753  11.662  1.00 52.17
ATOM   3426  N   ALA   448      43.804  27.387  13.584  1.00 53.51
ATOM   3427  CA  ALA   448      44.071  25.953  13.621  1.00 55.46
ATOM   3428  CB  ALA   448      43.273  25.306  14.745  1.00 55.02
ATOM   3429  C   ALA   448      43.751  25.263  12.300  1.00 57.02
ATOM   3430  O   ALA   448      44.599  24.564  11.726  1.00 57.18
ATOM   3431  N   VAL   449      42.523  25.457  11.825  1.00 58.39
ATOM   3432  CA  VAL   449      42.093  24.841  10.579  1.00 59.69
ATOM   3433  CB  VAL   449      40.571  24.977  10.382  1.00 59.67
ATOM   3434  CG1 VAL   449      40.152  24.262   9.112  1.00 60.28
ATOM   3435  CG2 VAL   449      39.833  24.384  11.577  1.00 59.48
ATOM   3436  C   VAL   449      42.821  25.482   9.403  1.00 60.70
ATOM   3437  O   VAL   449      42.903  24.898   8.321  1.00 61.00
ATOM   3438  N   ALA   450      43.361  26.677   9.627  1.00 61.41
ATOM   3439  CA  ALA   450      44.093  27.392   8.591  1.00 62.12
ATOM   3440  CB  ALA   450      43.981  28.889   8.814  1.00 62.32
ATOM   3441  C   ALA   450      45.558  26.973   8.606  1.00 63.02
ATOM   3442  O   ALA   450      46.437  27.748   8.217  1.00 62.75
ATOM   3443  N   CYS   451      45.807  25.744   9.061  1.00 64.03
ATOM   3444  CA  CYS   451      47.160  25.183   9.148  1.00 65.19
ATOM   3445  CB  CYS   451      47.530  24.440   7.850  1.00 65.75
ATOM   3446  SG  CYS   451      46.901  22.720   7.723  1.00 66.86
ATOM   3447  C   CYS   451      48.239  26.217   9.474  1.00 65.22
ATOM   3448  O   CYS   451      47.929  27.230  10.144  1.00 65.18
ATOM   3449  OXT CYS   451      49.398  25.979   9.073  1.00 65.50
ATOM   3450  C1  HEX     1      31.023  47.521  12.611  1.00 25.83
ATOM   3451  C2  HEX     1      32.239  47.182  11.801  1.00 25.25
ATOM   3452  C3  HEX     1      32.203  45.697  11.565  1.00 25.11
ATOM   3453  C4  HEX     1      32.071  44.939  12.862  1.00 24.99
ATOM   3454  C5  HEX     1      31.030  45.591  13.785  1.00 25.34
ATOM   3455  C6  HEX     1      30.772  44.921  15.126  1.00 25.58
ATOM   3456  O1  HEX     1      30.750  48.942  12.579  1.00 27.04
ATOM   3457  O2  HEX     1      32.183  47.912  10.609  1.00 24.71
ATOM   3458  O3  HEX     1      33.337  45.251  10.836  1.00 25.99
ATOM   3459  O4  HEX     1      31.699  43.621  12.545  1.00 25.85
ATOM   3460  O5  HEX     1      31.267  46.968  13.935  1.00 25.37
ATOM   3461  O6  HEX     1      31.835  45.222  16.009  1.00 27.23
ATOM   3462  C1  LIG     1      30.034  26.620   8.669  1.00 35.87
ATOM   3463  C2  LIG     1      29.909  27.259  10.064  1.00 34.82
ATOM   3464  C3  LIG     1      31.308  27.852  10.344  1.00 35.54
ATOM   3465  C4  LIG     1      32.212  27.447   9.148  1.00 35.52
ATOM   3466  C5  LIG     1      31.520  26.207   8.584  1.00 35.20
ATOM   3467  C6  LIG     1      33.670  27.245   9.637  1.00 36.33
ATOM   3468  C7  LIG     1      34.562  26.321   8.758  1.00 37.11
ATOM   3469  C8  LIG     1      35.946  26.832   8.778  1.00 36.91
ATOM   3470  N9  LIG     1      36.382  27.317   7.570  1.00 36.92
ATOM   3471  C10 LIG     1      37.668  27.907   7.331  1.00 36.42
ATOM   3472  N11 LIG     1      38.035  28.336   6.087  1.00 37.39
ATOM   3473  C12 LIG     1      39.058  28.930   6.462  1.00 36.99
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FIG. 4III

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ATOM   3474  C13 LIG     1      39.426  29.003   7.575  1.00 37.10
ATOM   3475  S14 LIG     1      38.681  28.342   8.700  1.00 37.86
ATOM   3476  O15 LIG     1      36.640  26.843   9.817  1.00 38.32
ATOM   3477  C16 LIG     1      34.538  24.890   9.296  1.00 37.59
ATOM   3478  C17 LIG     1      34.906  24.620  10.610  1.00 37.22
ATOM   3479  C18 LIG     1      34.658  23.346  11.130  1.00 38.09
ATOM   3480  N19 LIG     1      34.084  22.371  10.404  1.00 38.80
ATOM   3481  C20 LIG     1      33.729  22.598   9.128  1.00 38.90
ATOM   3482  C21 LIG     1      33.942  23.860   8.546  1.00 38.73
ATOM   3483  K1  K       1      32.471  32.037  -7.104  1.00 46.91
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FIG. 4JJJ

CRYSTALS OF GLUCOKINASE AND METHODS OF GROWING THEM

This application claims priority of Provisional application Serial No. 60/341,988, filed Dec. 19, 2001.

FIELD OF THE INVENTION

The invention relates to crystalline forms of Gluckokinase of sufficient size and quality to obtain structural data by X-ray crystallography and to methods of growing such crystals.

BACKGROUND OF THE INVENTION

Glucokinase (GK) is one of four hexokinases found in mammals [Colowick, S. P., in *The Enzymes*, Vol. 9 (P. Boyer, ed.) Academic Press, New York, N.Y., pages 1–48, 1973]. The hexokinases catalyze the first step in the metabolism of glucose, i.e., the conversion of glucose to glucose-6-phosphate. Glucokinase has a limited cellular distribution, being found principally in pancreatic β-cells and liver parenchymal cells. In addition, GK is a rate-controlling enzyme for glucose metabolism in these two cell types that are known to play critical roles in whole-body glucose homeostasis [Chipkin, S. R., Kelly, K. L., and Ruderman, N. B. in *Joslin's Diabetes* (C. R. Khan and G. C. Wier, eds.), Lea and Febiger, Philadelphia, Pa., pages 97–115, 1994]. The concentration of glucose at which GK demonstrates half-maximal activity is approximately 8 mM. The other three hexokinases are saturated with glucose at much lower concentrations (<1 mM). Therefore, the flux of glucose through the GK pathway rises as the concentration of glucose in the blood increases from fasting (5 mM) to postprandial (≈10–15 mM) levels following a carbohydrate-containing meal [Printz, R. G., Magnuson, M. A., and Granner, D. K. in *Ann. Rev. Nutrition* Vol. 13 (R. E. Olson, D. M. Bier, and D. B. McCormick, eds.), Annual Review, Inc., Palo Alto, Calif., pages 463–496, 1993]. These findings contributed over a decade ago to the hypothesis that GK functions as a glucose sensor in β-cells and hepatocytes (Meglasson, M. D. and Matschinsky, F. M. *Amer. J. Physiol.* 246, E1–E13, 1984). In recent years, studies in transgenic animals have confirmed that GK does indeed play a critical role in whole-body glucose homeostasis. Animals that do not express GK die within days of birth with severe diabetes while animals overexpressing GK have improved glucose tolerance (Grupe, A., Hultgren, B., Ryan, A. et al., *Cell* 83, 69–78, 1995; Ferrie, T., Riu, E., Bosch, F. et al., *FASEB J.*, 10, 1213–1218, 1996). An increase in glucose exposure is coupled through GK in β-cells to increased insulin secretion and in hepatocytes to increased glycogen deposition and perhaps decreased glucose production.

The finding that type II maturity-onset diabetes of the young (MODY-2) is caused by loss of function mutations in the GK gene suggests that GK also functions as a glucose sensor in humans (Liang, Y., Kesavan, P., Wang, L. et al., *Biochem. J.* 309, 167–173, 1995). Additional evidence supporting an important role for GK in the regulation of glucose metabolism in humans was provided by the identification of patients that express a mutant form of GK with increased enzymatic activity. These patients exhibit a fasting hypoglycemia associated with an inappropriately elevated level of plasma insulin (Glaser, B., Kesavan, P., Heyman, M. et al., *New England J. Med.* 338, 226–230, 1998). While mutations of the GK gene are not found in the majority of patients with type II diabetes, compounds that activate GK and, thereby, increase the sensitivity of the GK sensor system will still be useful in the treatment of the hyperglycemia characteristic of all type II diabetes. Glucokinase activators will increase the flux of glucose metabolism in β-cells and hepatocytes, which will be coupled to increased insulin secretion. Such agents would be useful for treating type II diabetes.

In an effort to elucidate the mechanisms underlying kinase activation, the crystal structure of such proteins is often sought to be determined. The crystal structures of several hexokinases have been reported. See, e.g. A. E. Aleshin, C. Zeng, G. P. Bourenkov, H. D. Bartunik, H. J. Fromm & R. B. Honzatko 'The mechanism of regulation of hexokinase: new insights from the crystal structure of recombinant human brain hexokinase complexed with glucose and glucose-6-phosphate' *Structure* 6, 39–50 (1998); W. S. Bennett, Jr. & T. A. Steitz 'Structure of a complex between yeast hexokinase A and glucose I. Structure determination and refinement at 3.5 Å resolution' *J. Mol. Biol.* 140, 183–209 (1978); and S. Ito, S. Fushinobu, I. Yoshioka, S. Koga, H. Matsuzawa & T. Wakagi 'Structural Basis for the ADP-Specificity of a Novel Glucokinase from a Hyperthermophilic Archaeon' *Structure* 9, 205–214 (2001). Despite these reports, researchers armed with the knowledge of how to obtain crystals of related hexokinases have attempted to obtain crystals of any mammalian Glucokinase without success.

SUMMARY OF THE INVENTION

Applicants have discovered protocols which allow crystallization of mammalian Glucokinase with or without a bound allosteric ligand. The crystal structure has been solved by X-ray crystallography to a resolution of 2.7 Å. See FIGS. **3** and **4**. Thus the invention relates to a crystalline form of Gluckokinase and a crystalline form of a complex of Glucokinase and an allosteric ligand. The invention further relates to a method of forming crystals of Glucokinase, with or without a bound allosteric ligand.

BRIEF DESCRIPTION OF THE FIGURES

FIG. **1** shows Glucokinase co-crystals having P6(5)22 symmetry.

FIG. **2** shows the amino acid sequence of an expressed Glucokinase used for crystallization.

FIG. **3** shows a ribbon diagram of the structure of Glucokinase colored according to secondary structure. Light blue represents α-helix, dark blue represents 3_{10}-helix, green represents β-sheet and orange is coil.

FIGS. **4**A–JJJ shows the atomic structure coordinates for Glucokinase bound to 3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-yl-propionamide.

DETAILED DESCRIPTION OF THE INVENTION

The present invention relates to crystalline forms of mammalian Glucokinase, with or without a ligand bound in the allosteric site, where the crystals are of sufficient quality and size to allow for the determination of the three-dimensional X-ray diffraction structure to a resolution of about 2.0 Å to about 3.5 Å. The invention also relates to methods for preparing and crystallizing the Glucokinase. The crystalline forms of Glucokinase, as well as information derived from their crystal structures can be used to analyze and modify glucokinase activity as well as to identify compounds that interact with the allosteric site.

The crystals of the invention include apo crystals and co-crystals. The apo crystals of the invention generally

comprise substantially pure Glucokinase. The co-crystals generally comprise substantially pure Glucokinase with a ligand bound to the allosteric site.

It is to be understood that the crystalline Glucokinases of the invention are not limited to naturally occurring or native Glucokinases. Indeed, the crystals of the invention include mutants of the native Glucokinases. Mutants of native Glucokinases are obtained by replacing at lest one amino acid residue in a native Glucokinase domain with a different amino acid residue, or by adding or deleting amino acid residues within the native polypeptide or at the N- or C-terminus of the native polypeptide, and have substantially the same three-dimensional structure as the native Glucokinase from which the mutant is derived.

By having substantially the same three-dimensional structure is meant having a set of atomic structure coordinates from an apo- or co-crystal that have a root mean square deviation of less than or equal to about 2 Å when superimposed with the atomic structure coordinates of the native Glucokinase from which the mutant is derived when at least about 50% to about 100% of the alpha carbon atoms of the native Glucokinase are included in the superposition.

In some instances, it may be particularly advantageous or convenient to substitute, delete and/or add amino acid residues to a native Glucokinase domain in order to provide convenient cloning sites in cDNA encoding the polypeptide, to aid in purification of the polypeptide, etc. Such substitutions, deleteions and/or additions which do not substantially alter the three dimensional structure of the native Glucokinase will be apparent to those having skills in the art.

It should be noted that the mutants contemplated herein need not exhibit glucokinase activity. Indeed, amino acid substitutions, additions or deletions that interfere with the kinase activity of the glucokinase but which do not significantly alter the three-dimensional structure of the domain are specifically contemplated by the invention. Such crystalline polypeptides, or the atomic structure coordinates obtained therefrom, can be used to identify compounds that bind to the native domain. These compounds may affect the activity or the native domain.

The derivative crystals of the invention generally comprise a crystalline glucokinase polypeptide in covalent association with one or more heavy metal atoms. The polypeptide may correspond to a native or a mutated Glucokinase. Heavy metal atoms useful for providing derivative crystals include, by way of example and not limitation, gold and mercury. Alternatively, derivative crystals can be formed from proteins which have heavy atoms incorporated into one or more amino acids, such as seleno-methionine substitutions for methionine.

The co-crystals of the invention generally comprise a crystalline Glucokinase polypeptide in association with one or more compounds at an allosteric site of the polypeptide. The association may be covalent or non-covalent.

Production of Polypeptides

The native and mutated glucokinase polypeptides described herein may be isolated from natural sources or produced by methods well known to those skilled in the art of molecular biology. Expression vectors to be used may contain a native or mutated Glucokinase polypeptide coding sequence and appropriate transcriptional and/or translational control signals. These methods include in vitro recombinant DNA techniques, synthetic techniques and in vivo recombination/genetic recombination. See, for example, the techniques described in Maniatis et al., 1989, *Molecular Cloning: A Laboratory Manual*, Cold Spring Harbor Laboratory, NY; and Ausubel et al., 1989, *Current Protocols in Molecular Biology*, Greene Publishing Associates and Wiley Interscience, NY.

A variety of host-expression vector systems may be utilized to express the Glucokinase coding sequence. These include but are not limited to microorganisms such as bacteria transformed with recombinant bacteriophage DNA, plasmid DNA or cosmid DNA expression vectors containing the Glucokinase coding sequence; yeast transformed with recombinant yeast expression vectors containing the Glucokinase coding sequence; insect cell systems infected with recombinant virus expression vectors (e.g. baculovirus) containing the Glucokinase coding sequence; plant cell systems infected with recombinant virus expression vectors (e.g., cauliflower mosaic virus, CaMV; tobacco mosiac virus, TMV) or transformed with recombinant plasmid expression vectors (e.g., Ti plasmid) containing the glucokinase coding sequence; or animal cell systems. The expression elements of these systems vary in their strength and specificities. Depending on the host/vector system utilized, any of a number of suitable transcription and translation elements, including constitutive and inducible promoters such as pL of bacteriophage μ, plac, ptrp, ptac (ptrp-lac hybrid promoter) and the like may be used; when cloning in insect cell systems, promoters such as the baculovirus polyhedrin promoter may be used; when cloingin in plant cell systems, promoters derived from the genome of plant cells (e.g., heat shock promoters; the promoter for the small subunit of RUBISCO; the promoter for the chlorophyll a/b binding protein) or from plant viruses (e.g., the 35 S RNA promoter of CaMV; the coat protein promoter of TMV) may be used; when cloning in mammalian cell systems, promoters derived from the genome of mammalian cells (e.g., metallothionein promoter) or from mammalian viruses (e.g., the adenovirus late promoter; the vaccinia virus 7.5 K promoter) may be used; when generating cell lines that contain multiple copies of the glucokinase coding sequence, SV40-, BPV- and EBV-based vectors may be used with an appropriate selectable marker.

Crystallization of Polypeptides and Characterization of Crystal Structure

The apo, derivative and co-crystals of the invention can be obtained by techniques well-known in the art of protein crystallography, including batch, liquid bridge, dialysis, vapor diffusion and hanging drop methods (see e.g. McPherson, 1982, *Preparation and Analysis of Protein Crystals*, John Wiley, NY; McPherson, 1990, *Eur. J. Biochem.* 189:1–23; Webber, 1991, *Adv. Protein Chem.* 41:1–36; Crystallization of Nucleic Acids and Proteins, Edited by Arnaud Ducruix and Richard Giege, Oxford University Press; Protein Crystallization Techniques, Strategies, and Tips, Edited by Terese Bergfors, International University Line, 1999). Generally, the apo- or co-crystals of the invention are grown by placing a substantially pure Gluckokinase polypeptide in an aqueous buffer containing a precipitant at a concentration just below that necessary to precipitate the protein. Water is then removed from the solution by controlled evaporation to produce crystallizing conditions, which are maintained until crystal growth ceases.

In a preferred embodiment of the invention, apo or co-crystals are grown by vapor diffusion. In this method, the polypeptide/precipitant solution is allowed to equilibrate in a closed container with a larger aqueous reservoir having a precipitant concentration optimal for producing crystals. Generally, less than about 10 μL of subtantially pure polypeptide solution is mixed with an equal volume of

reservoir solution, giving a precipitant concentration about half that required for crystallization. This solution is suspended as a droplet underneath a coverslip, which is sealed onto the top of a reservoir. The sealed container is allowed to stand, from one day to one year, usually for about 2–6 weeks, until crystals grow.

For crystals of the invention, it has been found that hanging drops containing about 2–5 μl of Glucokinase (9–22 mg/ml in 20 mM tris pH 7.1 measured at room temperature, 50 mM NaCl, 50 mM glucose, 10 mM DTT and optionally 0.2 mM EDTA) and an equal amount of reservoir solution (16–25% w/v polyethylene glycol with an average molecular weight from about 8000 to about 10000 Daltons, 0.1–0.2 M tris or bistris or Hepes or ammonium phosphate buffer, pH 6.9–7.5, 8–10 mM DTT, 0–30% saturated glucose) suspended over 0.5 to 1.0 mL reservoir buffer for about 3-4 weeks at 4–6° C. provided crystals suitable for high resolution X-ray structure determination. Particularly preferred conditions were: about 2–5 μl of Glucokinase (10 mg/ml in 20 mM tris pH 7.1 measured at room temperature, 50 mM NaCl, 50 mM glucose, 10 mM DTT and optionally 0.2 mM EDTA) and an equal amount of reservoir solution (22.5% w/v polyethylene glycol with an average molecular weight of about 10000 Daltons, 0.1 M tris pH 7.08, 10 mM DTT, 20% glucose) were suspended over 0.5 to 1.0 mL reservoir buffer for about 3–4 weeks at 4–6° C.

The optimum procedure for growing crystals large enough to collect data from involved first streaking 3–4 μl of protein solution on the coverslip, followed by streaking 3–4 μl of well solution across the elongated droplet of protein, forming a droplet shaped like the letter 'X'. Before discovering this crossed droplet technique, most droplets yielded showers of small crystals which were not large enough for data collection purposes. The crossed droplets allow gradients of protein and precipitating agent to form as the two solutions slowly mix, and the resulting kinetics of crystal nucleation and growth are optimal for the growth of a small number of large crystals in each crossed droplet. Simply mixing the protein and precipitant solutions together in a single round droplet often produced an overabundance of nuclei which grew to a final size too small for data collection purposes. Crystals usually appeared within 5 days of setup. The crystals grow in the form of hexagonal bipyramids, reaching dimensions of 0.2×0.2×0.4 mm typically, although larger crystals are often observed. FIG. **1** shows grown crystals.

Crystals may be frozen prior to data collection. The crystals were cryo-protected with either (a) 20–30% saturated glucose present in the crystallization setup, (b) ethanol added to 15–20%, (c) ethylene glycol added to 10–20% and PEG10,000 brought up to 25%, or (d) glycerol added to 15%. The crystals were either briefly immersed in the cryo-protectant or soaked in the cryo-protectant for periods as long as a day. Freezing was accomplished by immersing the crystal in a bath of liquid nitrogen or by placing the crystal in a stream of nitrogen gas at 100 K.

The mosaic spread of the frozen crystals could sometimes be reduced by annealing, wherein the stream of cold nitrogen gas is briefly blocked, allowing the frozen crystal to thaw momentarily before re-freezing in the nitrogen gas stream. Another technique which was sometimes helpful in data collection was to center one of the ends of the hexagonal bipyramid in the x-ray beam, rather than the mid portion of the crystal. The mosaic spread could sometimes be reduced by this technique.

Diffraction data typically extending to 2.7 Å was collected from the frozen crystals at the synchrotron beamline X8C of the National Synchrotron Light Source in Brookhaven, N.Y. Under optimum conditions, data extending to 2.2 Å was recorded. See FIGS. **3** and **4** for solution. The space group of the crystals was determined to be P6(5)22 during the course of the solution of the crystal structure. The crystals have unit cell dimensions a=b=79.62+/−0.60 Å, c=321.73+/−3.70 Å, α=β=90°, γ=120°. The crystals are in a hexagonal system with P6(5)22 symmetry.

Of course, those having skill in the art will recognize that the above-described crystallization conditions can be varied. Such variations may be used alone or in combination, and include polypeptide solutions containing polypeptide concentrations between 1 mg/mL and 60 mg/mL, any commercially available buffer systems which can maintain pH from about 6.5 to about 7.6, Tris-HCl concentrations between 10 mM and 200 mM, dithiothreitol concentrations between 0 mM and 20 mM, substitution of dithiothreitol with beta mercapto ethanol or other art-recognized equivalents, or substitution of glucose with other sugars known to bind to Glucokinase; and reservoir solutions containing polyethylene glycol concentrations between about 10% and about 30%, polyethylene glycol average molecular weights between about 1000 and about 20,000 daltons, any commercially available buffer systems which can maintain pH from about 6.5 to about 7.6, dithiothreitol concentrations between 0 mM and 20 mM, substitution of dithiothreitol with beta mercapto ethanol or other art-recognized —SH group containing equivalents, or substitution of glucose with other sugars known to bind to Glucokinase, and temperature ranges between 4 and 20° C.

Derivative crystals of the invention can be obtained by soaking apo or co-crystals in mother liquor containing salts of heavy metal atoms, according to procedures known to those of skill in the art of X-ray crystallography.

Co-crystals of the invention can be obtained by soaking an apo crystal in mother liquor containing a ligand that binds to the allosteric site, or can be obtained by co-crystallizing the Glucokinase polypeptide in the presence of one or more ligands that bind to the allosteric site. Preferably, co-crystals are formed with a glucokinase activator disclosed in U.S. Pat. No. 6,320,050; U.S. patent application Ser. No. 09/532,506 filed Mar. 21, 2000; U.S. patent application Ser. No. 09/675,781 filed Sep. 28, 2000; U.S. patent application Ser. No. 09/727,624, filed Dec. 1, 2000; U.S. patent application Ser. No. 09/841,983, filed Apr. 25, 2001; U.S. patent application Ser. No. 09/843,466, filed Apr. 26, 2001; U.S. patent application Ser. No. 09/846,820, filed May 1, 2001; U.S. patent application Ser. No. 09/846,821, filed May 1, 2001; U.S. patent application Ser. No. 09/905,152, filed Jul. 13, 2001; U.S. patent application Ser. No. 09/924,247, filed Aug. 8, 2001; U.S. Provisional Pat. Appl. No. 60/251,637, filed Dec. 6, 2000; or U.S. Provisional Pat. Appl. No. 60/318,715, filed Sep. 13, 2001, each of which is incorporated herein by reference.

Methods for obtaining the three-dimensional structure of the crystalline glucokinases described herein, as well as the atomic structure coordinates, are well-known in the art (see, e.g., D. E. McRee, Practical Protein Crystallography, published by Academic Press, San Diego (1993), and references cited therein).

Uses of the Crystals and Atomic Structure Coordinates

The crystals of the invention, and particularly the atomic structure coordinates obtained therefrom, have a wide variety of uses. For example, the crystals and structure coordinates described herein are particularly useful for identifying compounds that activate Glucokinases as an approach towards developing new therapeutic agents.

The structure coordinates described herein can be used as phasing models in determining the crystal structures of additional native or mutated glucokinases, as well as the structures of co-crystals of such glucokinases with allosteric inhibitors or activators bound. The structure coordinates, as well as models of the three-dimensional structures obtained therefrom, can also be used to aid the elucidation of solution-based structures of native or mutated glucokinases, such as those obtained via NMR. Thus, the crystals and atomic structure coordinates of the invention provide a convenient means for elucidating the structures and functions of glucokinases.

For purposes of clarity and discussion, the crystals of the invention will be described by reference to specific Glucokinase exemplary apo crystals and co-crystals. Those skilled in the art will appreciate that the principles described herein are generally applicable to crystals of any mammalian Glucokinase, including, but not limited to the Glucokinase of FIG. **2**.

Definitions

As used herein, "allosteric site" refers in general to any ligand binding site on a mammalian Glucokinase other than the active site of the enzyme.

As used herein, "apo crystal" refers to crystals of mammalian Glucokinase formed without a bound allosteric ligand.

As used herein, "allosteric ligand" refers to any molecule which specifically binds an allosteric site on a mammalian Glucokinase.

EXAMPLES

Example 1

Expression and Purification of Glucokinase

Expression of GK

Glucokinase (GK) was expressed as a glutathione S-transferase (GST) fusion protein in *Escherichia coli*. The amino-acid sequence of the fusion protein is given in FIG. **2**. The expression construct is based on the pGEX-3X vector from Pharmacia, as described in Y. Liang, P. Kesavan, L. Wang, K. Niswender, Y. Tanizawa, M. A. Permutt, M. A. Magnuson, F. M. Matschinsky, *Biochem. J.* 309, 167 (1995). The construct codes for one of the two liver isozymes of human GK. The GST tag is at the N-terminus of the construct, and is separated from the coding sequence for GK by a Factor Xa cleavage site. After purification of the GST fusion protein, the GST fusion tag was removed with Factor Xa protease, which also removes five residues from the N-terminus of GK.

Purification of GK

E. coli cells expressing GST-GK were suspended in lysis buffer (50 mM tris, 200 mM NaCl, 5 mM EDTA, 5 mM DTT, 1% NP-40, pH 7.7) in the presence of protease inhibitors, incubated with lysozyme at 200 μ/ml for 30 minutes at room temperature, and sonicated 4×30 sec. at 4° C. After centrifugation to remove insoluble material, the supernatant was loaded onto glutathione-Sepharose, washed with lysis buffer and then with lysis buffer minus NP-40. GST-GK was eluted with lysis buffer (minus NP-40) containing 50 mM D-glucose and 20 mM glutathione. The eluted protein was concentrated and dialyzed into 20 mM tris, 100 mM NaCl, 0.2 mM EDTA, 50 mM D-glucose, 1 mM DTT, pH 7.7. Factor Xa was added at a protein ratio of 1:100 GST-GK followed by the addition of $CaCl_2$ to 1 mM, and the sample was incubated at 4° C. for 48 hours. The sample was added to glutathione Sepharose and the unbound fraction collected and concentrated. The sample was then incubated with benzamidine Sepharose to remove Factor Xa, and the unbound fraction was collected and loaded on a Q Sepharose column equilibrated with 25 mM bis-tris propane, 50 mM NaCl, 5 mM DTT, 50 mM D-glucose and 5% glycerol (pH 7.0). The protein was eluted with a NaCl gradient from 50–400 mM. Fractions containing purified GK were pooled and concentrated and filtered.

Example 2

Formation of Apo Crystal

4 μl of glucokinase and 4 μl of precipitant were mixed and equilibrated against the precipitant solution at 4° C. The glucokinase solution consisted of 22 mg/ml glucokinase prepared in Example 1 in 20 mM hepes pH 7.5, 50 mM NaCl, 10 mM DTT, and 50 mM glucose. The precipitant consisted of 22.5% PEG10000, 0.1 M tris pH 7.08, 10 mM DTT, 20% glucose; the precipitant solution contained seed crystals in order to microseed the droplets. Crystals appeared in the droplets after leaving the crystallization plates at 4° C.

Example 3

Formation of Co-crystal with 3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-yl-propionamide

3(a):

4 μl of glucokinase and 4 μl of precipitant were mixed and equilibrated against the precipitant solution at 4° C. The glucokinase solution consisted of 13 mg/ml glucokinase prepared in Example 1 in 20 mM tris pH 7.0, 50 mM NaCl, 10 mM DTT, 50 mM glucose, and the glucokinase activator 3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-yl-propionamide at a concentration 5 times that of the protein. The precipitant consisted of 22.5% PEG10000, 0.1 M tris pH 7.08, 10 mM DTT, 20% glucose. Crystals appeared in the droplets after leaving the crystallization plates at 4° C.

3(b):

Alternatively, crystals were grown as in Example 3(a) with the following changes: instead of 4 μl glucokinase and 4 μl precipitant, 2 μl of each were used; the glucokinase solution contained 11 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of 22.5% PEG10000 as precipitant 18% PEG8000 was used; the precipitant solution contained seed crystals in order to microseed the droplets.

3(c):

In another alternative, crystals were grown as in Example 3(a) with the following changes: instead of 4 μl glucokinase and 4 μl precipitant, 2 μl of each were used; the glucokinase solution contained 11 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of 22.5% PEG10000 as precipitant 20% PEG8000 was used; the precipitant solution contained seed crystals in order to microseed the droplets.

3(d):

In yet another alternative, crystals were grown as in Example 3(a) with the following changes: instead of 4 μl glucokinase and 4 μl precipitant, 2 μl of each were used; the glucokinase solution contained 12 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of 22.5% PEG10000 as precipitant 16% PEG10000 was used; glucose was not present as a component of the precipitant; the precipitant solution contained seed crystals in order to microseed the droplets.

3(e):

In still another alternative, crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 11 mg/ml glucokinase in tris buffer at pH 7.1 instead of 7.0; the glucokinase solution included 0.2 mM

EDTA; in place of 22.5% PEG10000 as precipitant 25% PEG10000 was used.

3(f):

In still another alternative, crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 11 mg/ml glucokinase in tris buffer at pH 7.1 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of 22.5% PEG10000 as precipitant 21.25% PEG10000 was used; in place of tris buffered at pH 7.08 in the precipitant tris buffered at pH 7.52 was used.

3(g):

In still another alternative, crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 12 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of tris buffered at pH 7.08 in the precipitant, hepes buffered at pH 6.89 was used; in place of 20% glucose in the precipitant, 200 mM glucose was used.

3(h):

In still another alternative, crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 12 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of 0.1 M tris buffered at pH 7.08 in the precipitant, 0.2 M ammonium phosphate buffered at pH 7.03 was used; in place of 20% glucose in the precipitant, 200 mM glucose was used.

3(i):

In still another alternative, crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 10 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of 22.5% PEG10000 as precipitant, 20% PEG10000 was used; in place of tris buffered at pH 7.08 in the precipitant, tris buffered at pH 7.05 was used; in place of 10 mM DTT in the precipitant, 8 mM DTT was used; glucose was not present as a component of the precipitant.

3(j):

In still another alternative, crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 12 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of 22.5% PEG10000 as precipitant, 22% PEG8000 was used; glucose was not present as a component of the precipitant; the precipitant solution contained seed crystals in order to microseed the droplets.

3(k):

In still another alternative, crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 11 mg/ml glucokinase in tris buffer at pH 7.1 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of 20% glucose in the precipitant, 30% glucose was used.

Example 4

Formation of Co-crystal with N-(5-Bromo-pyridin-2-yl)-2-(3-chloro-4-methanesulfonyl-phenyl)-3-cyclopentyl-propionamide

Crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 9 mg/ml glucokinase in tris buffer at pH 7.1 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of the glucokinase activator of Example 3(a), the glucokinase solution contained the glucokinase activator N-(5-Bromo-pyridin-2-yl)-2-(3-chloro-4-methanesulfonyl-phenyl)-3-cyclopentyl-propionamide; in place of 20% glucose in the precipitant, 200 mM glucose was used.

Example 5

Formation of Co-crystal with 2-(3-Chloro-4-methanesulfonyl-phenyl)-3-cyclopentyl-N-(5-trifluoromethyl-pyridin-2-yl)-propionamide

Crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 10 mg/ml glucokinase in tris buffer at pH 7.1 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of the glucokinase activator of Example 3(a), the glucokinase solution contained the glucokinase activator 2-(3-Chloro-4-methanesulfonyl-phenyl)-3-cyclopentyl-N-(5-trifluoromethyl-pyridin-2-yl)-propionamide; in place of 22.5% PEG10000 as precipitant, 21.25% PEG1000 was used.

Example 6

Formation of Co-crystal with (2S)-2-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionylamino]-thiazole-4-carboxylic Acid Methyl Ester

Crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 10 mg/ml glucokinase in tris buffer at pH 7.1 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of the glucokinase activator of Example 3(a), the glucokinase solution contained the glucokinase activator (2S)-2-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionylamino]-thiazole-4-carboxylic acid methyl ester; in place of 22.5% PEG10000 as precipitant, 21.25% PEG10000 was used; in place of tris buffered at pH 7.08 in the precipitant, bistris buffered at pH 7.0 was used.

Example 7

Formation of Co-crystal with (2S)-{2-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionylamino]-thiazol-5-yl}-oxo-acetic Acid Ethyl Ester

Crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 10 mg/ml glucokinase in tris buffer at pH 7.1 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of the glucokinase activator of Example 3(a), the glucokinase solution contained the glucokinase activator (2S)-{2-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionylamino]-thiazol-5-yl}-oxo-acetic acid ethyl ester; in place of 22.5% PEG10000 as precipitant, 21.25% PEG10000 was used.

Example 8

Formation of Co-crystal with (2S)-{3-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionyl]-ureido}-acetic Acid Methyl-ester

Crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 9 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of the glucokinase activator of Example 3(a), the glucokinase solution contained the glucokinase activator (2S)-{3-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionyl]-ureido}-acetic acid methylester; in place of 20% glucose in the precipitant, 200 mM glucose was used.

Example 9

Formation of Co-crystal with (2S)-1-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionyl]-3-(3-hydroxy-propyl)-urea

Crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 14 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of the glucokinase activator of Example 3(a), the glucokinase solution contained the glucokinase activator (2S)-1-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionyl]-3-(3-hydroxy-propyl)-urea; in place of 20% glucose in the precipitant, 200 mM glucose was used.

Example 10

Formation of Co-crystal with (2S)-{3-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionyl]-ureido}-acetic Acid Ethyl Ester

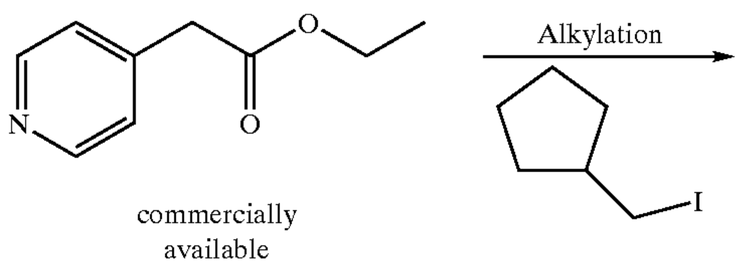
Crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 14 mg/ml

glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of the glucokinase activator of Example 3(a), the glucokinase solution contained the glucokinase activator (2S)-{3-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionyl]-ureido}-acetic acid ethyl ester; in place of tris buffered at pH 7.08 in the precipitant, tris buffered at pH 7.05 was used.

Example 11

Synthesis of 3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-yl-propionamide

3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-yl-propionamide can be prepared using well-known organic synthesis techniques according to the following reaction scheme:



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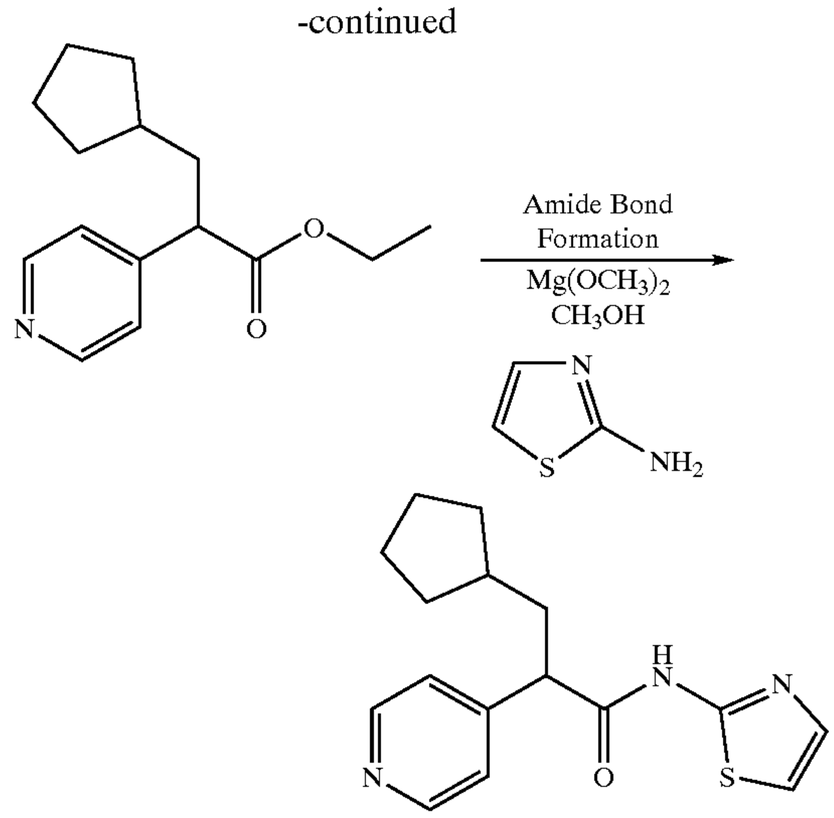

3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-yl-propionamide is useful as an allosteric activator of Glucokinase and to assist the formation of co-crystals of Glucokinase.

SEQUENCE LISTING

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<211> LENGTH: 692
<212> TYPE: PRT
<213> ORGANISM: Escherichia coli

<400> SEQUENCE: 1

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            20                  25                  30

Tyr Glu Arg Asp Glu Gly Asp Lys Trp Arg Asn Lys Lys Phe Glu Leu
        35                  40                  45

Gly Leu Glu Phe Pro Asn Leu Pro Tyr Tyr Ile Asp Gly Asp Val Lys
    50                  55                  60

Leu Thr Gln Ser Met Ala Ile Ile Arg Tyr Ile Ala Asp Lys His Asn
65                  70                  75                  80

Met Leu Gly Gly Cys Pro Lys Glu Arg Ala Glu Ile Ser Met Leu Glu
                85                  90                  95

Gly Ala Val Leu Asp Ile Arg Tyr Gly Val Ser Arg Ile Ala Tyr Ser
            100                 105                 110

Lys Asp Phe Glu Thr Leu Lys Val Asp Phe Leu Ser Lys Leu Pro Glu
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Met Leu Lys Met Phe Glu Asp Arg Leu Cys His Lys Thr Tyr Leu Asn
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Val Val Leu Tyr Met Asp Pro Met Cys Leu Asp Ala Phe Pro Lys Leu
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Thr Phe Gly Gly Gly Asp His Pro Pro Lys Ser Asp Leu Ile Glu Gly
    210                 215                 220

Arg Gly Ile His Met Pro Arg Pro Arg Ser Gln Leu Pro Gln Pro Asn
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Ser Gln Val Glu Gln Ile Leu Ala Glu Phe Gln Leu Gln Glu Glu Asp
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Lys Leu His Pro Ser Phe Lys Glu Arg Phe His Ala Ser Val Arg Arg
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Leu Thr Pro Ser Cys Glu Ile Thr Phe Ile Glu Ser Glu Glu Gly Ser
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Met Leu Gly Gln
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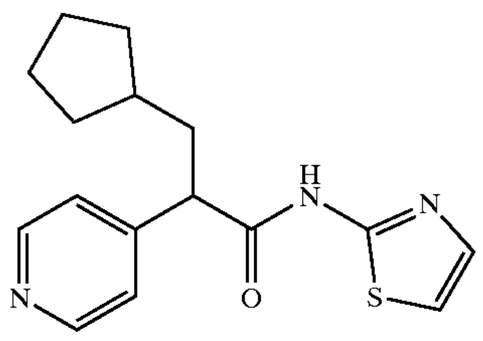
We claim:

1. The compound



and pharmaceutically acceptable salts thereof.

* * * * *

UNITED STATES PATENT AND TRADEMARK OFFICE

CERTIFICATE OF CORRECTION

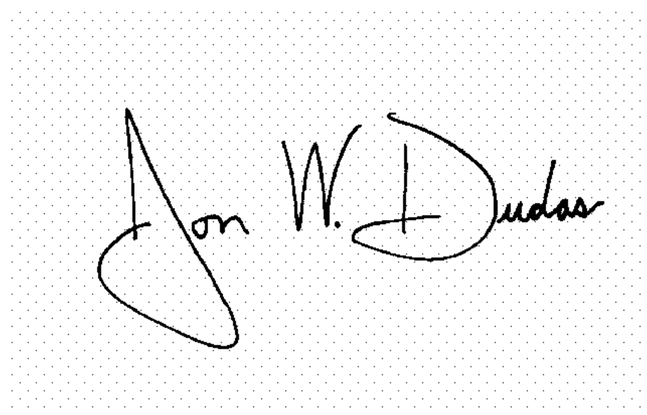
PATENT NO. : 6,911,545 B2
DATED : June 28, 2005
INVENTOR(S) : Corbett et al.

It is certified that error appears in the above-identified patent and that said Letters Patent is hereby corrected as shown below:

Title page,
Item [73], Assignee, "**Hoffman-La Roche Inc.**, Nutley, NJ" should be -- **Hoffmann-La Roche Inc.**, Nutley, NJ --.

Signed and Sealed this

Sixth Day of September, 2005



JON W. DUDAS
Director of the United States Patent and Trademark Office